SCATTERING OF PHONONS FROM A SUBSTITUTIONAL IMPURITY IN CUBIC LATTICES

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1. Scattering of phonons from a substitutional impurity; Proc. Phys. Soc. (London) 85, 1223 (1965)
   (Co-author: J. Mahanty)
2. Scattering of phonons from a substitutional impurity in body centred cubic and face centred cubic lattices, Proc. Phys. Soc. (London) 87, 689 (1966)
   (Co-author: J. Mahanty)
3. Green function integrals for simple cubic lattice; Technical Report No. 3/65, Deptt. of Physics, Indian Institute of Technology, Kanpur, India.
4. Green function integrals for body centred cubic lattice; Technical Report No. 6/65, Department of Physics, Indian Institute of Technology, Kanpur, India.

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ABSTRACT

The scattering of phonons from a substitutional impurity in cubic lattices is studied in detail with the help of Green function technique used by Lifshitz and Montroll and Potts. Exact solutions for scattering amplitude are found explicitly and the scattering amplitude is expanded in terms of partial waves characterized by the irreducible representations of the point group of the lattice. The scattering cross sections are found in the limit of long waves showing Rayleigh type of scattering in absence of resonances which are taken care of by the resonance denominators.

Specific examples of the scattering of phonons from substitutional impurities in simple cubic, body centred cubic and face centred cubic lattices are worked out in detail. Curves are given showing the dependence of resonance frequencies on parameters characterizing changes in mass and force constant. The long wavelength behavior of the scattering process is discussed and the total cross sections are found using optical theorem in this limit. The dependence of the scattering cross sections on the direction of incidence is shown by noting the different partial wave contributions for different directions of incidence. The inverse of mean free path for phonons due to scattering by substitutional impurities is found in the long wavelength limit. It is shown to be proportional to ω^4 with resonance possibilities and the interference terms between partial waves characterized by different irreducible representationsare given explicitly. Phonon scattering from a substitional impurity in a

diatomic simple cubic lattice is also discussed and curves are drawn showing the dependence of resonance frequencies upon the parameters characterizing changes in mass and force constant.

At the end, a model of body centred cubic lattice is considered in which the polarization of phonons is taken into account in the description of the scattering process, which is shown to depend upon the direction of incidence as well as the state of polarization of the incident phonons. The dispersion law for the model does not go over to the Debye model in the limit of long waves and consequently the dependence of the number of partial waves contributing to the scattering cross section even in the limit of long waves depends upon the incident direction and polarization of incident phonons. The result for the isotope defect case in the limit of long waves differs from that calculated by assuming Debye model by a numerical factor which depends upon the direction of incidence. A comparison is made between this and the so called scalar models.

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CHAPTER I

INTRODUCTION

The problem of scattering of phonons by a substitutional impurity was first treated by I.M. Lifshitz[1-2] whose pioneering work[3] on the problem of Dynamic Theory of Non-ideal crystal lattice is well known. It has subsequently been discussed by many workers[4-17] including the author [18-19]. Most of the fundamental concepts and methodological aspects of the problem are present in Lifshitz's work. It has been shown that the problem can be worked out exactly using Green function techniques. The perturbation due to impurity may be large but the range of this perturbation is assumed to be quite small within the crystal. The principal result is that the perturbed region surrounding the impurity appears as a separate system whose energy levels depend upon the energy spectrum of the host lattice. If the perturbation is sufficiently large, an impurity level may lie outside the band, with a long lifetime since there are no states in the neighbourhood into which it can decay. On the other hand for moderate perturbations the impurity level will lie inside the band with a finite probability of decay. The latter level has profound effects on the scattering of phonons from the impurity.

As an example Lifshitz, considered the case of an isotope defect and the scattering of phonons from it. He obtained the expression for the scattering amplitude by expanding the proper Green function for large distances. The behavior of this process in the limit of long waves are also discussed. Montroll and Potts [4-5] independently considered the problem in the same way as Lifshitz did. They also showed that the case of diatomic lattices can be handled by the formalism for mono-atomic lattices by performing the so called M^* transformation. Although Lifshitz noticed the fact that by the introduction of a substitutional impurity the translational symmetry of the lattice is destroyed and only the point group symmetry remains, the idea of expanding the phonon scattering amplitude in terms of partial waves characterised by the irreducible representations of the point group of the lattice was developed by others [9,20-21].

The rest of the work in this field has been mostly matters of detail. The literature is extensive but the notations are uncorrelated, some times to the extent of confusing the reader. Maradudin[7] has discussed the details and refinements of the problem on several occasions. Takeno[10], Callaway[9], Wagner[12], Krumhansl[16-17] and Thoma and Ludwig[13] have also considered the details of the problem with its implications on the evaluation of thermal conductivity due to scattering of phonons from substitutional impurities. In many of these the idea of resonant scattering has been stressed. Krumhansl and Matthew[17] considered the problem in a one dimensional model in a rather complete way, and have demonstrated interference between different partial waves in the expression for relaxation time. This has been elaborated for three dimensions in the present work. Elliot and Taylor[11] solved the problem by using double time Green function technique in an elegant way. Recently Klein [14-15] has given a completely general formulation of the problem within the framework of the quantum mechanical formal theory of scattering. Several importent aspects like the optical theorem and orthonormality of the solutions have been discussed in this work. Wagner[12] has discussed the case of molecular impurities by introducing the molecular Green function.

There has been considerable overlaping among the approaches and results of the various workers mentioned above. The overall picture at present is that we have made substantial progress in understanding the details of the problem, but this by no means is complete and final. Experiments in this field has lagged behind theory and new experiments may reveal more details than has been known hitherto. The main source of experimental information on scattering of phonons from substitutional impurities at present is the low temperature thermal conductivity data. By analysing this, Walker and Pohl[22-23] were able to infer the presence of resonance scattering leading to the deviation from Klemens' result[24]. Baumann[25] and Klein[26] also arrived at similar conclusions. Very recently Huebener[27] has estimated the scattering cross section for phonons scattered from vacancies by measuring the change in thermoelectric power in Platinum. A remark relevant to these experiments is that usually the impurities do not always go into substitutional sites. They sometimes go into interstitial positions so that the results have to be interpreted cautiously.

There is a great deal of similarity among the problems of scattering of phonons, band electrons and spin waves from substitutional impurities. This has been explored by Callaway[9] in detail. Formalisms identical to that for the phonon scattering for the other two cases have been developed by various workers[20-21,28-30].

In this dissertation scattering of phonons from substitutional impurities in some three dimensional lattice models are considered in detail. The scattering amplitudes are expanded in terms of partial waves characterised by different irreducible representations of the point group of the lattice and the scattering cross sections are evaluated in the limit of long waves. The question of resonant scattering of phonons in the optical band of a diatomic simple cubic lattice is discussed. At the end a model of body centred cubic lattice is considered in which the polarisation of phonons is taken into account in the description of the scattering process. The question of the dependence of the scattering process on the direction of incident phonons is also examined. Finally the implications of a departure from Debye model in the limit of long waves is discussed.

CHAPTER II

GENERAL FORMULATION

§ 2.1 Introduction,

The theory of scattering of phonons from substitutional impurities started with efforts concentrated on isotopic impurities involving only a change in mass. It was further believed that the first Born approximation results were adequate to describe the process[24], but this assumption was soon abandoned [8,10-11]. The low temperature thermal conductivity experiments by Klein[26], Walker and Pohl[22-23] and Baumann[25] showed the inadequacy of first Born approximation results and the necessity of including resonant scattering which can be done by solving the problem exactly. They further showed that the rather simple case of isotope defect was also inadequate. One should consider the scattering of phonons from point defects characterized by changes in mass as well as force constant. Moreover one should look for exact solutions rather than perturbation approximations. We consider such an approach to the problem of scattering of phonons from a substitutional impurity in the present work.

Some other investigators have considered this approach as already mentioned in the last chapter. Many other workers[4,31] have been interested in the determination of only the localized modes due to a 'general substitutional impurity' by which we will mean, throughout this work, a substitutional impurity characterized by changes in mass as well as force constants. However this determination of localized modes can be achieved in a natural way from the solution of the general scattering problem.

The simplest model for the scattering of phonons from a general substitutional impurity has been considered by Krumhansl and Matthew[17]. Although they consider a one-dimensional problem, the qualitative conclusions derived are quite instructive and useful. Klein[14] develops a t-matrix formalism which is applicable to three dimensional crystals. This has been extended further by his latest work[15] which contains many important theorems and an averaging procedure for a distribution of defects. It is a self consistent formalism applicable to many models and yields results that are identical to those of the simple formalism described below (when applied to the same models), except that it is perhaps easier to extract numbers out of the latter than from the former formalism. Also the explicit detailed treatment of the resonance denominators in the latter formalism facilitates the investigation of resonances and localized modes.

Before discussing the present formalism it is worthwhile to note that this scattering problem is analogous to the potential scattering in ordinary quantum mechanics except for two important differences. It is a particular case of the more general problem of scattering of quasi-particles in crystalline solids which has been studied by Callaway[9]. One of the differences is due to the fact that the dispersion law giving the wave number dependence of the single particle energy reveals the typical band structure involving both an upper and a lower bound to the energy. This permits the possibility of occurrence of bound states both above and below the optical bands and above the acoustic band, depending on the nature of the scatterer. Moreover for the scattering process both the incident and the scattered particles have their admissible energies limited to the band. The wave number is also limited to lie within the first Brillouin Zone. The other difference is related to the symmetry of the problem. The interaction due to the scatterer usually possesses the symmetry of the point group of the crystal rather than the spherical symmetry of the potentials studied in the theory of potential scattering. This feature necessitates a change in the method of partial wave analysis of the scattering amplitude which now has to be decomposed in terms of partial waves characterized by the irreducible representations of the point group of the lattice.

The present formalism is perhaps mathematically simpler and less formal than those cited above. The scattering amplitudes and their partial wave expansions are explicitly presented and the optical theorem in the usual form is employed to demonstrate the non-central effects of a general perturbation. The solution is exact and includes resonant scatterings. The long wavelength limit is found easily. The interference between terms corresponding to different partial waves can also be seen explicitly in the evaluation of relaxation times.

§ 2.2 The Model

The formalism developed here depends upon a number of assumptions. The first is the adiabatic approximation in which it is assumed that the electrons instantenously take up a configuration appropriate to that of the displaced nuclei and that the change of energy of the electrons in the distorted lattice contributes to an effective internuclear potential. This is quite plausible for the vibrations in the acoustic modes that we will deal with. The other important approximation is the harmonic approximation. Since the harmonic force constants assumed here may have a temperature dependence, we are in effect assuming a pseudo-harmonic approximation which is adequate for low temperature properties.

Here we consider a monoatomic lattice and investigate cases where the question of polarization does not enter into the picture. The so called 'scalar models' belong to this category. In addition there are models other than these scalar models which do not mix polarization such as the one discussed in the next chapter. The discussion of polarization is taken up in chapter V of the present work and a discussion of a diatomic lattice in the next chapter shows how the results for the monoatomic lattices can be easily carried over to the case of diatomic lattices by using the so called M^* transformation[5]. With slight modifications, the results obtained here can be carried over to the case of the scattering of spin waves [28–30] and the scattering of band electrons[20–21] from substitutional impurities in the lattice.

The lattice under consideration has N atoms of mass M each which are coupled to their neighbours through harmonic force constants. The time independent equations of motion can be written as,

$$\hat{A}\underline{U} - (M\omega^2)\,\underline{U} = 0 \qquad (2.1)$$

where $\hat{A}$ is the force constant matrix of dimensions $N \times N$ and $\underline{U}$ is the N-dimensional vector whose elements are the one component displacements (scalar field) of atoms from their equilibrium sites with a time dependence of the form $\exp(-i\omega t)$.

The matrix $\hat{A}$ can be shown to be cyclic and hence its eigenvectors $\underline{U}_o(\underline{k})$ have elements of the form

$$U_o(\underline{k}, \underline{R}) = N^{-\frac{1}{2}} \exp(i\underline{k}.\underline{R}) \qquad (2.2)$$

where $\underline{R}$ denotes the lattice sites with reference to a given origin. The vector $\underline{k}$ (with N different values) specifies the eigenvectors and the corresponding eigenvalues. $U_o(\underline{k}, \underline{R})$ has the form of a running wave or a phonon propagating with a wave vector $\underline{k}$. Substituting equation (2·2) in equation (2.1), one gets the eigenvalues of $\hat{A}$ which give the frequency squared as a function of $\underline{k}$ i,e the dispersion law which is written as $\omega^2(\underline{k})$ and this has both an upper and a lower bound defining the band. The distinct values of $\underline{k}$ lie within the first Brillouin Zone. The eigenvectors $\underline{U}_o(\underline{k})$ satisfy the orthogonality and closure properties in an obvious way

$$\sum_{\underline{k}} U_o^*(\underline{k}, \underline{R}') U_o(\underline{k}, \underline{R}) = \delta_{\underline{R}, \underline{R}'}$$

$$\text{and} \quad \sum_{\underline{R}} U_o^*(\underline{k}', \underline{R}) U_o(\underline{k}, \underline{R}) = \delta_{\underline{k}, \underline{k}'} \qquad (2.3)$$

These properties of $\hat{A}$ and its eigenvectors are direct consequences of the cyclic boundary conditions imposed on the lattice.

§ 2.3.The perturbed lattice,

Let a substitutional impurity be put into the lattice. This changes the mass of the atom at the substituted site to $M + \Delta M$ and the coupling of this impurity atom to its nearest neighbours is given by the changed harmonic force constant $\gamma + \Delta\gamma$ where $\Delta\gamma$ denotes the change in the normal value γ. Thus the impurity affects the site it occupies plus its neighbours whose number is determined by the range of interaction. All these sites including that of the impurity atom are called the sites affected by the perturbation. In most of the cases these affected sites can be assumed to have the symmetry of the point group of the lattice with the impurity site as the point left invariant under the operations of this point group. Strictly speaking, the resulting symmetry group of the system will be the intersection of the point group of the lattice and the symmetry group of the perturbation. What we are assuming here in effect amounts to believing that the symmetry group of the perturbation has at least all the elements of the point group of the lattice.

Then the displacements of all the atoms at the affected sites form a representation space of the point group of the lattice in which the reducible representation Γ of the point group can be decomposed in terms of the irreducible representations $\Gamma^{(\nu)}$ of the point group as

$$\Gamma = \sum_{\nu} a_{\nu} \, \Gamma^{(\nu)} \qquad (2.4)$$

where a_{ν} are zero or integers. The above representation space will be called the Γ-space.

The equations of motion of the perturbed lattice can be written as

$$\hat{A} \, \underline{U} - (M \omega^2) \, \underline{U} = \hat{P} \, \underline{U} \qquad (2.5)$$

where the N x N perturbation matrix $\hat{P}$ has non-vanishing elements only in the Γ-space and can be partitioned into the form

$$\hat{P} = \begin{pmatrix} \hat{p} & 0 \\ 0 & 0 \end{pmatrix} \qquad (2.6)$$

where the matrix $\hat{p}$ is of dimensions $n \times n$ and n is the number of lattice sites affected by the perturbation, i.e. the dimensionality of the Γ-space.

The solution of equation (2.5) outside the unperturbed band will give the discrete frequencies corresponding to bound states in potential scattering. They are the localised modes of the lattice with impurity. The scattering state solutions are obtained for values of ω^2 within the unperturbed band and can be written as satisfying an equation of the form ,

$$\underline{U} = \underline{U}_0 - \hat{G}\hat{P}\underline{U} \qquad (2.7)$$

where the Green function matrix $\hat{G}$ is defined as ,

$$\hat{G} = -(\hat{A} - M\omega^2 \hat{I})^{-1} \qquad (2.8)$$

where $\hat{I}$ is the unit matrix. $\underline{U}_0$ is the unperturbed solution having the same eigenvalue as $\underline{U}$ and this is always possible in a large lattice, because the frequencies form a continuum.

The matrix elements of $\hat{G}$ can be written explicitly as,

$$G(\omega^2, \underline{R}, \underline{R}') = -\frac{1}{M}\sum_{\underline{k}} \frac{U_0(\underline{k}, \underline{R})\, U_0^*(\underline{k}, \underline{R}')}{\omega^2(\underline{k}) - \omega^2} \qquad (2.9)$$

The summation over $\underline{k}$ is over the first Brillouin Zone.

The disadvantage of the use of such Green functions for the three- dimensional problems is that they must be calculated numerically even for the simplest cases if quantitative results are desired. However some numerical tables are available[20,28,32–33] and recently a simplified numerical method based on the Fourier series expansion has been given by Mahanty[34]. These Green functions also occur in problems of scattering of band electrons and spin waves from substitutional impurities.

Using equation (2.2) for $U_0(\underline{k}, \underline{R})$ in equation (2.9), the Green function matrix elements can be written as,

$$G(\omega^2, \underline{R}, \underline{R}') = -\frac{1}{MN} \sum_{\underline{k}} \frac{\exp\{-i\,\underline{k}.(\underline{R}'-\underline{R})\}}{\omega^2(\underline{k}) - \omega^2} \tag{2.10}$$

The matrix $\hat{G}$ is cyclic like the matrix $\hat{A}$ and hence its elements depend upon the difference $\underline{R} - \underline{R}'$.

Now the equation (2.7) can be solved for $\underline{U}$. The first Born approximation solution consists of writing $\underline{U}_0$ for $\underline{U}$ on the right hand side of equation (2.7). Thus the first Born approximation solution of equation (2.7) reads,

$$\underline{U} = \underline{U}_0 - \hat{G}\hat{P}\,\underline{U}_0 \tag{2.11}$$

This shows that $\underline{U}$ is equal to the incident wave $\underline{U}_0$ plus another part which we wish to represent an outgoing wave for our scattering problem. This can be achieved by writing equation (2.10) in the form,

$$G(\omega^2, \underline{R}, \underline{R}')_{m} = -\frac{1}{MN} \sum_{\underline{k}} \frac{\exp\{i\underline{k}.(\underline{R}'-\underline{R}')\}}{\omega^2(\underline{k}) - \omega^2 - i\epsilon} \tag{2.12}$$

with $\epsilon \to 0$.

In the usual way the second Born approximation solution will be,

$$\underline{U} = \underline{U}_0 - \hat{G}\hat{P}\,\underline{U}_0 - (\hat{G}\hat{P})^2\,\underline{U}_0 \tag{2.13}$$

and so on. Thus one gets the perturbation series solution. But this does not show resonance in the scattering process. Also for large perturbations such a series has convergence problems.

Instead of equation (2.13) we wish to solve equation (2.7) exactly. In a formal way, the exact solution reads,

$$\underline{U} = \underline{U}_o - \hat{G}\,\hat{P}(\,\hat{I} + \hat{G}\,\hat{P})^{-1}\,\underline{U}_o \qquad (2.14\ )$$

The orthonormality of solutions of the form of equation(2.14) has been discussed in detail by Klein [15] and others [7]. We now proceed to describe the operational procedure for obtaining an exact solution of equation (2.7) like the one given by equation (2.14).

§ 2.4 Solution for the scattering amplitude

In order to obtain an explicit solution we partition $\underline{U}$ in the form,

$$\underline{U} = \begin{pmatrix} \underline{u} \\ \underline{U}_{(1)} \end{pmatrix} \qquad (2.15)$$

where $\underline{u}$ is a n-dimensional vector in the Γ-space corresponding to the nonvanishing partition $\hat{p}$ of $\hat{P}$ described in equation (2.6). In a similar fashion, the matrix $\hat{G}$ and the vactor $\underline{U}_o$ can be partitioned into ,

$$\hat{G} = \begin{pmatrix} \hat{g} & \hat{G}_{(12)} \\ \hat{G}_{(21)} & \hat{G}_{(22)} \end{pmatrix} \qquad (\ 2.16)$$

$$\text{and} \quad \underline{U}_o = \begin{pmatrix} \underline{uo} \\ \underline{U}_{(01)} \end{pmatrix} \qquad (\ 2.17)$$

where $\hat{g}$ is n x n matrix in Γ-space corresponding to the partition $\hat{p}$ and $\underline{uo}$ is in Γ-space corresponding to $\underline{u}$.

Let us define the N - dimensional vectors $\underline{S}$ and $\underline{S}_0$ by,

$$\underline{S} = \hat{P}\,\underline{U} \tag{2.18}$$

and

$$\underline{S}_0 = \hat{P}\,\underline{U}_0 \tag{2.19}$$

By multiplying the partitioned form of $\hat{P}$ given by equation (2.6) and using equations (2.15) and (2.17) for the partition of $\underline{U}$ and $\underline{U}_0$ one gets,

$$\underline{S} = \begin{pmatrix} \underline{s} \\ \underline{0} \end{pmatrix} \tag{2.20 }$$

and

$$\underline{S}_0 = \begin{pmatrix} \underline{s}_0 \\ \underline{0} \end{pmatrix} \tag{2.21 }$$

where $\underline{s} = \hat{p}\,\underline{u}$ and $\underline{s}_0 = \hat{p}\,\underline{u}_0$ (2.22)

Now multiplying equation (2.7) by $\hat{P}$ on both the sides by the left, one gets

$$\hat{P}\,\underline{U} = \hat{P}\,\underline{U}_0 - \hat{P}\,\hat{G}\,\hat{P}\,\underline{U}$$

or

$$\underline{S} = \underline{S}_0 - \hat{P}\,\hat{G}\,\underline{S} \tag{2.23}$$

which in the partitioned form reads,

$$\begin{pmatrix} \underline{s} \\ \underline{0} \end{pmatrix} = \begin{pmatrix} \underline{s}_0 \\ \underline{0} \end{pmatrix} - \begin{pmatrix} \hat{p} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{g} & \hat{G}(12) \\ \hat{G}(21) & \hat{G}(22) \end{pmatrix} \begin{pmatrix} \underline{s} \\ \underline{0} \end{pmatrix}.$$

whence the reduced equation for $\underline{s}$ is ,

$$\underline{s} = \underline{s}_0 - \hat{p}\,\hat{g}\,\underline{s} \tag{2.24}$$

so that

$$\underline{s} = (\hat{I} + \hat{p}\hat{g})^{-1}\,\underline{s}_0 \tag{2.25}$$

or

$$\underline{s} = (\hat{I} + \hat{p}\,\hat{g})^{-1}\,\hat{p}\,\underline{u}_0 \tag{2.26}$$

Thus the matrix involved in equation (2.26) is only of the dimensions n x n. For a given case one knows $\hat{p}$ and $\hat{g}$ explicitly. But still to find the inverse of ($\hat{I} + \hat{p}\,\hat{g}$) in a straight-forward manner is often very tedious. To ease this task, one can employ a unitary matrix $\hat{V}$ which block diagonolizes $\hat{I} + \hat{p}\,\hat{g}$. One could even think in terms of a unitary matrix which completely diagonolizes it, but such a matrix is difficult to obtain. On the other hand there exists a unitary matrix $\hat{V}$ which can be found easily by group theoretical procedure and which can block diagonolize $\hat{p}$ and $\hat{g}$ and hence ($\hat{I} + \hat{p}\,\hat{g}$) into blocks of quite manageable dimensions. Then it is very easy to find the inverse of ($\hat{I} + \hat{p}\,\hat{g}$). The number of such blocks, the dimensionality of each block and the number of identical blocks for the block diagonolization by such a $\hat{V}$ matrix can be known by applying the following theorem from group theory to the decomposition of Γ given by equation (2.4). The theorem[35] states that if $\Gamma = \sum_{\nu} a_{\nu}\, \Gamma^{(\nu)}$ and if $\Gamma^{(\nu)}$ has the dimensionality n_{ν} then in the block diagonal form there will be n_{ν} identical a_{ν} x a_{ν} blocks.

Further if one writes the block diagonal matrix $\hat{V}^{+}(\hat{I} + \hat{p}\,\hat{g})^{-1}\hat{V}$ as the sum of matrices in which only one out of these blocks which corresponds to a certain irreducible representation is non-zero, then using each of them one can evaluate vectors $\underline{s}_{\nu}$ whose sum will be $\underline{s}$. This decomposition of $\underline{s}$ is equivalent to projecting the different symmetry adapted functions out of $\underline{s}$, which belong to different irreducible representations of the point group. This in turn leads to the partial wave expansion of the scattering amplitude. Thus the matrix $\hat{V}$ found by group theoretic procedure not only facilitates the evaluation of the inverse matrix in equation (2.26) but also leads to partial wave expansion of the scattering amplitude as shown below . The evaluation of such matrices is described in the Appendix III.

Thus let,

$$\hat{T} = \hat{V}^{+} (\hat{I} + \hat{p}\,\hat{g}) \hat{V} \tag{2.27}$$

where $\hat{T}$ is the block diagonal matrix with h blocks. It is very easy to find the inverse of $\hat{T}$ since this has blocks of very small dimensions. Let $\hat{T}^{-1}$ be written in the block form,

$$\hat{T}^{-1} = \begin{pmatrix} \hat{t}_1 & 0 & \cdots\cdots \\ 0 & \hat{t}_2 & \cdots\cdots \\ \cdot\;\cdot\;\cdot & \cdot\;\cdot\;\cdot\;\cdot & \cdot\;\cdot\;\cdot\;\cdot \\ & & \cdots\;\hat{t}_h \end{pmatrix} \tag{2.28}$$

Now each of the blocks $\hat{t}_1$, $\hat{t}_2$, ... $\hat{t}_h$ correspond to a unique irreducible representation of the point group of the lattice. We define the matrices $\hat{M}_\nu$ such that $\hat{M}_\nu$ has non-vanishing elements in the ν th block only, i.e

$$\hat{M}_\nu = \begin{pmatrix} 0 & \cdot\;\cdot\;\cdot & \cdot\;\cdot\;\cdot\;\cdot \\ \cdot\;\cdot & \cdot\;\cdot\;\cdot & \cdot\;\cdot\;\cdot\;\cdot \\ \cdot\;\cdot & \hat{t}_\nu & \cdots\cdots \\ \cdot\;\cdot & \cdot\;\cdot\;\cdot & \cdot\;\cdot\;\cdot\;\cdot \end{pmatrix} \tag{2.29}$$

$$\text{and} \quad \hat{T}^{-1} = \sum_{\nu=1}^{h} \hat{M}_\nu \tag{2.30}$$

Thus $(\hat{I} + \hat{p}\,\hat{g})^{-1} = \hat{V}\,\hat{T}^{-1}\,\hat{V}^{+} = \sum_{\nu=1}^{h} \hat{V}\,\hat{M}_\nu\,\hat{V}^{+}$ and $\underline{g} = \sum_{\nu=1}^{h} \underline{g}_\nu$

where $\underline{s}_\nu = \hat{V}\,\hat{M}_\nu\,\hat{V}^+\,\hat{p}\,\underline{u}_o$ (2.31)

One obtains the same result if one block diagonolizes $\hat{p}$ as well by the $\hat{V}$ matrix and writes it ~~as~~ the sum of matrices like $\hat{M}_\nu$, multiplies the νth blocks of these and defines $\underline{s}_\nu$ as $\underline{s}_\nu = \hat{V}\,(\hat{M}\,\hat{p}\,)_\nu\,\hat{V}^+\,\underline{u}_o$.

The $\underline{s}_\nu$ defined like this belong to particular rows of particular irreducible representations of the point group of the lattice. This identification can be done by identifying the columns of $\hat{V}$ - matrix which is done during its evaluation. One would get the same result if one finds $\underline{s}$ by direct inversion in equation (2.26) and then applies the group theoretic projection operators to $\underline{s}$ to find the $\underline{s}_\nu$ that belong to given rows of given irreducible representations.

Now going back to equation (2.20) one finds that $\underline{S}$ can be written as ,

$$\underline{S} = \sum_{\nu=1}^{h} \underline{S}_\nu \qquad \text{where} \quad \underline{S}_\nu = \begin{pmatrix} \underline{s}_\nu \\ \underline{0} \end{pmatrix} \qquad (2.32)$$

and then equation (2.7) reads

$$\underline{U} = \underline{U}_o - \sum_{\nu=1}^{h} \hat{G}\,\underline{s}_\nu \qquad (2.33)$$

This equation is the analogue of the familiar partial wave analysis result of the theory of potential scattering. Here the number of terms is finite and equals the number of submatrices in the block diagonal form of $\hat{p}$ which in turn depends upon the range of interaction due to the impurity and the point group of the lattice. In component form, equation (2.33) becomes,

$$U(\underline{k}, \underline{R}) = U_o(\underline{k},\underline{R}) - \sum_{\nu=1}^{h} \sum_{\underline{R}_n} G(\omega^2, \underline{R},\underline{R}_n)\, S_\nu\, (\underline{k},\underline{R}_n) \qquad (2.34)$$

where $\underline{R}_n$ refers to the lattice sites affected by the perturbation including the impurity site and the summation is over all of them. These are quite small in number and the non-vanishing elements of $\underline{S}_\nu$ refer to these only. Using equation (2.10) for $G(\omega^2, \underline{R},\underline{R}_n)$ one gets for large $\underline{R}$, as shown in the Appendix II,

$$\lim_{R\to\infty} G(\omega^2, \underline{R},\underline{R}_n) \simeq - \sum_{\underline{k}_o} g(\underline{k}_o) \exp\left[i\underline{k}_o.(\underline{R}-\underline{R}_n)\right] / |\underline{R}|$$

and consequently equation (2.34) gives

$$U(\underline{k},\underline{R}) = U_o(\underline{k},\underline{R}) + \sum_{\text{all } \underline{k}_o} g\,(\underline{k}_o)\, \frac{\exp}{|\underline{R}|N^{\frac{1}{2}}}(i\ \underline{k}_o.\underline{R}) \sum_{\nu} F_\nu\,(\underline{k},\underline{k}_o) \qquad (2.35)$$

where $F_\nu\,(\underline{k},\underline{k}_o)$ is a function of the components of $\underline{k}$ and $\underline{k}_o$. Here $\underline{k}_o$ is such that $\omega^2(\underline{k}_o) = \omega^2$ with $\nabla_k \omega^2\,(\underline{k})\Big|_{\underline{k}_o}$ having the direction of $\underline{R}$. For symmetry directions in the lattice $\underline{k}_o$ represents the direction of the scattered wave and often there are not more than one $\underline{k}_o$ satisfying $\omega^2(\underline{k}_o) = \omega^2$ along these directions.

Equation (2.35) gives us the desired solution with the outgoing spherical waves characterized by $\exp(i\ \underline{k}_o.\underline{R})/|\underline{R}|$ whose co-efficient is the scattering amplitude. This point has been discussed in detail by Callaway[9]. Thus the scattering amplitude is

$$f\ (\underline{k},\underline{k}_o) = \sum_{\nu=1}^{h} g(\underline{k}_o)\ F_\nu\,(\underline{k},\underline{k}_o) \qquad (2.36)$$

and the desired partial wave expansion can be written as,

$$f\,(\underline{k},\underline{k}_0) = \sum_{\mu} f_{\mu}\,(\underline{k},\underline{k}_0) \qquad (2.37)$$

where $f_{\mu}(\underline{k},\underline{k}_0) = \sum_{\nu} g(\underline{k}_0)\, F_{\nu}\,(\underline{k},\underline{k}_0)$ with ν summed over n_{μ} values where n_{μ} is the dimensionality (degeneracy) of the μ th irreducible representation.

For incident waves along the symmetry axes in the lattice, it is quite easy to evaluate the forward scattering amplitudes. Thus one sets $\underline{k} = \underline{k}_0$ in equation (2.36) to get the forward scattering amplitude.

In describing the details of the partial wave analysis we shall follow the classification of S,P,D,F etc. type of waves according to the Wigner's scheme described by Callaway[9] and given in detail in Appendix III. Thus having obtained the scattering amplitude one can evaluate the differential scattering cross section in the usual way. Also the total scattering cross section can be found by integrating over the angles. Such a procedure is cumbersome in general, but in the limit of long waves it can be done for simple cases. In this limit the constant frequency surfaces become spherical for the model under discussion and hence $\nabla_k \omega^2(\underline{k})\Big|_{\underline{k}_0}$ lies along $\underline{k}_0$. Then $\underline{k}_0$ represents the direction of propagation as well as the direction of observation for all directions of incident waves which are characterized by $\underline{k}$ and the angle between $\underline{k}$ and $\underline{k}_0$ is the scattering angle.

As mentioned above, one can evaluate the forward scattering amplitude for incidence along symmetry directions. For such directions of incidence one can evaluate the total scattering cross section σ_T

by using the optical theorem. That the optical theorem holds good for the type of scattering under consideration has been discussed by Thoma and Ludwig[13] and Klein[15]. We feel that the optical theorem given by Thoma and Ludwig[13] which can be derived using the results for $\sigma_D(\theta)$ given by Callaway[9], is sufficient for the present work and it is given by

$$\sigma_T = \frac{4\pi \left| \omega^2|_{11}(\underline{k})\ \omega^2|_{22}(\underline{k}) \right|^{\frac{1}{2}}}{\left| \mathrm{grad}_{\underline{k}}\ \omega^2(\underline{k}) \right|}\ \mathrm{Im}\left[f(\underline{k},\underline{k})\ \exp\left\{\frac{i\pi}{4}(\epsilon_1+\epsilon_2-2)\right\}\right] \tag{2.38}$$

where $f(\underline{k},\underline{k})$ is the forward scattering amplitude. Here $\omega^2|_{ii}(\underline{k})$ means the second derivatives of $\omega^2(\underline{k})$ in $\underline{k}$ space with respect to a coordinate system that is perpendicular to $\mathrm{grad}_{\underline{k}}\,\omega^2(\underline{k})$ and diagonalizes the tensor $\omega^2|_{ij}(\underline{k})$, $(i, j = 1,2)$ and ϵ_i is given by sgn $\omega^2|_{ii}(\underline{k})$. However, it must be remarked here that from the experimental point of view one is interested not in the total scattering cross section but the momentum transfer cross section which is required for the calculation of thermal conductivity. This is discussed in the following section. The limit of long waves is very relevant for such calculations because it is a plausible approximation for explaining the results for low temperature experiments. Also the optical theorem in this limit takes the usual form of $\sigma_T = \frac{4\pi}{k}\ \mathrm{Im}\left[f(\underline{k},\underline{k})\right]$ for the model under discussion.

It is clear that resonant scatterings are included in the above calculations. Equation (2.26) shows that $\underline{s}$ has det $\left|\hat{I} + \hat{p}\,\hat{g}\right|$ in the denominator. Further from equation (2.27) it follows that det $\left|\hat{I} + \hat{p}\,\hat{g}\right|$ = det $\left|\hat{T}\right|$ which in turn is the product of the determinants of the blocks of $\hat{T}$ which correspond to different symmetry types. Thus det $|\hat{I} + \hat{p}\hat{g}| = \det|\hat{T}| = \Pi_j b_j$ where b_j is the determinant of the jth block which corresponds to a given symmetry. These are exhibited explicitly in the next two chapters. These sub-determinants b_j occur as denominators in the expressions for $f_\mu(\underline{k},\underline{k}_0)$ or equivalently one can speak of $\Pi_j b_j$ occurring in the denominator of $f(\underline{k},\underline{k}_0)$. In general b_j are complex within the band and can be written as $b_j = b_{j,r} + i\, b_{j,i}$, where $b_{j,r}$ and $b_{j,i}$ are real. Moreover these are functions of the incident energy E. Outside the band $b_{j,i} \equiv 0$ and b_j are completely real. Localized modes appear when any of the sub-determinants b_j vanish outside the band. This can be seen by multiplying equation (2.5) by $\hat{G}$ from the left to get $\underline{U} = -\hat{G}\hat{P}\underline{U}$. Here we do not have a $\underline{U}_0$ because we consider ω^2 outside the band. Now following the partitioning described by equations (2.15), (2.16) and (2.6), we get

$$\underline{u} = -\hat{g}\hat{p}\underline{u} \qquad (2.39)$$

This is an eigenvalue, eigenvector problem in Γ-space. Solution of this equation exists for ω^2 determined by the condition det $|\hat{I} + \hat{g}\hat{p}| = \Pi_j b_j = 0$. These are the localized modes of vibration whose amplitude falls off rapidly with distance from the impurity and these have been discussed in detail by many workers[4,31]. Since b_j are identified into different symmetry types, one speaks of localized modes of different symmetries and degeneracies corresponding to the b_j that vanishes to give rise to these modes. Since we evaluate the factors b_j explicitly in the present formalism, it becomes very easy to investigate the existence of localized modes.

Inside the band, the real part $b_{j,r}$ may vanish for certain values of incident energy E. It will correspond to a resonance in the scattering amplitude provided that the imaginary part $b_{j,i}$ and $\frac{d\,b_{j,r}}{dE}$ have the same sign and their ratio is small. This additional requirement comes from the consideration of the density of phonon states of the perturbed lattice as shown below. We do not use the density of phonon states elsewhere although it can be evaluated easily using the above formalism. The density of phonon states for the perturbed lattice can be written as $n_p = -\frac{1}{\pi}\,\mathrm{Im}(\mathrm{Tr}\,\hat{G}')$ where the perturbed Green function G' is given by

$$\hat{G}' = \hat{G} - \hat{G}\hat{P}\,(\hat{I} + \hat{G}\hat{P})^{-1}$$

whence the contribution of the impurity to the density of states can be written as

$$\Delta n = -\frac{1}{\pi}\,\mathrm{Im}\left[\frac{d}{dE}\ln\left(\det\left|\hat{I} + \hat{G}\hat{P}\right|\right)\right] \qquad (2.40)$$

But due to the partition of $\hat{P}$ into the only non-vanishing small block $\hat{p}$, one has

$$\det\left|(\hat{I} + \hat{G}\hat{P})\right| = \det\left|\hat{I} + \hat{g}\hat{p}\right| = \prod_j b_j$$

where we also use the fact that $(\hat{I} + \hat{p}\hat{g})^T = (\hat{I} + \hat{g}\hat{p})$ and that the transposition does not alter the value of the determinant. Then equation (2.40) becomes

$$\Delta n = -\frac{1}{\pi}\sum_j \mathrm{Im}\left[\frac{\frac{db_j}{dE}}{b_j}\right]$$

$$= \frac{1}{\pi}\sum_j \left[\frac{b_{j,i}\frac{db_{j,r}}{dE} - b_{j,r}\frac{db_{j,i}}{dE}}{(b_{j,r})^2 + (b_{j,i})^2}\right] \qquad (2.41)$$

But at resonance, $b_{j,r} = 0$ and $\Delta n_j = \frac{1}{\pi}\left[\left(\frac{d}{dE} b_{j,r}\right) / b_{j,i}\right]$ (2.42)

is the contribution from a particular impurity state, which when compared with the resonance formula

$$n\,(E) = \frac{1}{\pi}\,\frac{\Gamma_\omega}{(E-E_o)^2 + \Gamma_\omega^{\,2}}$$

which at resonance reads

$$n(E) = \frac{1}{\pi\,\Gamma_\omega}$$

gives the result for the level width

$$\Gamma_\omega = \frac{b_{j,i}}{b'_{j,r}} \qquad (2.43)$$

Here prime denotes the derivative with respect to E. For resonance Γ_ω should be positive. The smaller the Γ_ω, the sharper is the resonance.

§ 2.5 Relation with the transport phenomena:

So far only one defect at a particular lattice site has been considered. In actual practice one has a number of such defects randomly distributed over the lattice sites. These can even migrate and interact with each other. But at low temperatures and small concentrations, it is perhaps not a bad assumption that very little migration of defects takes place. We want to consider the effect of scattering under these conditions upon the heat transport phenomenan, but since we will not be interested in the explicit evaluation of thermal conductivity in the present work, the details will be omitted.

The problem of thermal conductivity can be tackled in two ways.

The conventional method is that of writing down the Boltzmann transport equation[36,37] and solving it in the Kinetic theory approximation. The other more recent method is through the so called Kubo[38] formula. This has been used recently by Behera and Deo[39] among others to calculate the thermal conductivity. However we confine ourselves to a discussion of the conventional method.

In the conventional method one has two distinct approaches which give the same result. One is the classical method in which one writes the energy flow equation along the lines indicated by Choquard[40], evaluating the various quantities for the perturbed system. The other is the quantum approach through transition probabilities and scattering cross sections. Since in the present formalism one can evaluate the scattering cross sections, we discuss here this latter approach. One starts with a Boltzmann equation for the number of phonons N_k with momentum $\underline{k}$ and studies its time evolution through the equation of the form

$$\left(\frac{\partial N_k}{\partial t}\right)_{\text{drift}} = -\left(\frac{\partial N_k}{\partial t}\right)_{\text{coll.}} \qquad (2.44)$$

During thermal conduction, the left hand side is due to the temperature gradient and has the form

$$\underline{v}_k \cdot \text{grad } T \left(\frac{dN_k}{dT}\right)$$

whereas the right hand side is due to the scattering for the present case. In the relaxation time approximation one writes

$$\left(\frac{\partial N_k}{\partial t}\right)_{\text{coll.}} = \frac{N_k^0 - N_k}{\tau(k)} \qquad (2.45)$$

which shows that in absence of the temperature gradient, the deviation from equilibrium in the mode $\underline{k}$ damps out exponentially in the characteristic time $\tau(k)$. With this one can solve the Boltzmann equation (2.44) for N_k and calculate the thermal conductivity. In terms of heat capacity $C(k)$ and the group velocity $\underline{v}$, the expression for thermal conductivity is

$$K = \frac{V}{(2\pi)^3} \int d^3k \, \tau(k) \, C(k) \, v^2 \cos^2\theta \qquad (2.46)$$

where V is the volume, θ is the angle between $\underline{v}$ and grad T and the integration is over the first Brillouin zone. Defining the mean free path $\Lambda(k) = \tau(k) v$, one has

$$K = \frac{V}{(2\pi)^3} \int d^3k \, \Lambda(k) \, v \, C(k) \cos^2\theta \qquad (2.47)$$

and $\Lambda(k)$ is given by[41]

$$\frac{1}{\Lambda(k)} = 2\pi N_c \int_0^{\pi} (1 - \cos\theta) \, \sigma_D(\theta) \sin\theta \, d\theta \qquad (2.48)$$

where N_c is the concentration (small) of the defects, $\sigma_D(\theta)$ is the differential cross section at polar angle θ. The weightage $(1-\cos\theta)$ measures the relative change in the component of the momentum along the initial direction of motion. The quantity

$$\sigma_n = 2\pi \int_0^{\pi} (1-\cos\theta) \, \sigma_D(\theta) \sin\theta \, d\theta \qquad (2.49)$$

is sometimes called the momentum transfer cross section. If $\sigma_D(\theta)$ is independent of θ as is the case for scattering from isotopic impurities, when the scattering is entirely S wave type, then σ_n equals the total cross section which can also be evaluated by using optical theorem. Of special importance is the long wave behavior of $\Lambda(k)$. Since $\sigma_D(\theta)$ contains resonance denominators, the quantity $\Lambda(k)$ registers a small value at the resonance in $\sigma_D(\theta)$. This in turn implies a smaller value of the thermal conductivity K than when resonance is absent. Thus the resonance in $\sigma_D(\theta)$ implies a 'dip' in the thermal conductivity curve.

An interesting feature of equation (2.48) is the interference between the terms of different symmetries. In particular terms of different inversion symmetries, (or parities) namely the 'gerade' and the 'ungerade' terms show interference. This is seen very easily in the limit of long waves where one has for example $f(\underline{k},\underline{k}_o) = f_g + f_u \cos\theta$ with f_g and f_u independent of θ. Then $\sigma_D = f^* (\underline{k},\underline{k}_o)\, f\, (\underline{k},\underline{k}_o)$

$$= |f_g|^2 + |f_u|^2 \cos^2\theta + (f_g f_u^* + f_u f_g^*) \cos\theta$$

whence by equation (2.49)

$$\sigma_n = 4\pi \left[|f_g|^2 + |f_u|^2/3 \right] - \frac{4\pi}{3} (f_g f_u^* + f_u f_g^*) \qquad (2.50)$$

The second term on the right hand side shows the above mentioned interference. This is shown more explicitly in the next chapter. It demonstrates the importance of the weightage factor (1-cos θ) in equation (2.48). This point has also been discussed by Krumhansl and Matthew[17].

Equation (2.48) shows another important result that for small concentrations for which the multiple scatterings from the defects can be neglected, the result for N_D defects is just N_D times the result for a single defect. If one starts from the consideration of random distribution of defects at small concentrations and averages out the various quantities, one arrives at this result as has been discussed by Klein[15] and Vashishta[30]. Thus the single impurity problem which appears too academic to begin with, is relevant to the physical situation under certain circumstances.

CHAPTER III

SIMPLE CUBIC LATTICE

§ 3.1. The Model:

In this chapter we consider a specific model and discuss the specific results in an explicit form. This model of a monoatomic simple cubic lattice with equal central and noncentral harmonic force constants has been discussed by Montroll and Potts[4]. There are N atoms of mass M each. The harmonic force constant γ characterizes both the central and non-central forces between the nearest neighbours only. This equality of central and non-central forces enables one to discuss the problem without bringing in the question of polarization. With lattice constant a and Cartesian unit vectors $\underline{e}_i$, the lattice sites have co-ordinates

$$\underline{R} = \ell a \underline{e}_1 + m a \underline{e}_2 + n a \underline{e}_3 \qquad (3.1)$$

where ℓ, m and n are integers. We shall use either $\underline{R}$ or (ℓ,m,n) to specify a lattice site. The cartesian components of displacement from equilibrium of the atom at site (ℓ,m,n) are given by $x_{\ell mn}$, $y_{\ell mn}$ and $z_{\ell mn}$. As discussed by Montroll and Potts[4], one can think of any of these $x_{\ell mn}$ for example as a parameter associated with each lattice point (ℓ,m,n) and then this model is equivalent to a scaler model. With this it is possible to write the equations of motion of the perfect lattice in the form of equation (2.1)

$$\hat{A}\underline{U} - M\omega^2\underline{U} = 0 \qquad (3.1)$$

where $\hat{A}$ has the matrix elements given by

$$A(\ell mn, \ell' m'n') = \gamma \Big[6\, \delta_{\ell \ell'}\, \delta_{m,m'}\, \delta_{n,n'} - \delta_{m,m'}\, \delta_{n,n'} \left\{ \delta_{\ell+1,\ell'} + \delta_{\ell-1,\ell'} \right\} - \delta_{\ell \ell'}\, \delta_{n,n'} \left\{ \delta_{m+1,m'} + \delta_{m-1,m'} \right\} - \delta_{\ell,\ell'}\, \delta_{m,m'} \left\{ \delta_{n+1,n'} + \delta_{n-1,n'} \right\} \qquad (3.2)$$

and

$$U(\underline{k}, \ell mn) = X_{\ell mn}$$

The same matrix element $A(\ell mn, \ell' m'n')$ will describe the motion when $U(\underline{k}, \ell mn)$ are chosen to be $Y_{\ell mn}$ or $Z_{\ell mn}$.

The plane wave solutions corresponding to equation (2.2) are

$$U_o(\underline{k}, \ell mn) = N^{-\frac{1}{2}} \exp\left[i (k_1 \ell + k_2 m + k_3 n) \right] \qquad (3.3)$$

which correspond to the dispersion law

$$\omega^2(\underline{k}) = \frac{2\gamma}{M} \left(3 - \sum_{j=1}^{3} \cos k_j\right) \qquad (3.4)$$

Now let the defect atom be situated at the origin of the coordinate system. It has a mass $M + \Delta M$ and is coupled to its nearest neighbours through force constant $\gamma + \Delta\gamma$. The perturbation matrix $\hat{P}$ has non-vanishing elements only when the indices refer to the impurity site and its nearest neighbours. Denoting the nearest neighbour vectors by $\underline{R}_n$, the non-vanishing elements of $\hat{P}$ are

$$P(\underline{0},\underline{0}) = \Delta M \omega^2 - 6\Delta\gamma \;, \; P(\underline{R}_n, \underline{R}_n) = -\Delta\gamma$$

and

$$P(\underline{0},\underline{R}_n) = P(\underline{R}_n,\underline{0}) = \Delta\gamma \qquad (3.5)$$

Here $\underline{R}_n$ can have components (± 1, 0,0), (0,± 1, 0) and (0,0,± 1).

§ 3.2. The partial wave analysis:

As described in Appendix III, the reducible representation of the cubic group O_h in the space of the affected lattice sites (Γ -space) reduces in the usual notation[42] to

$$\Gamma_S = 2A_{1g} + F_{1u} + E_g \tag{3.6}$$

This leads to the unitary matrix $\hat{V}_s$ given explicitly in Appendix III. Now using the procedure outlined in the last chapter one can find the scattering amplitude. Here we follow the notation for the Green function integrals described in Appendix I for the simple cubic lattice. Also the matrices $\hat{p}$ and $\hat{g}$ are explicitly written with same indices for rows and columns as are used to label the rows and columns of $\hat{V}_s$ in Appendix III. With these the elements of block diagonal form of $(\hat{I}+\hat{p}\hat{g})^{-1}$, namely the $\hat{t}_\nu$ matrices of equation (2.28) are given by

$$\hat{t}_1 = \frac{\Delta\gamma}{F_s}\begin{pmatrix} Q & -6^{\frac{1}{2}}H \\ -6^{\frac{1}{2}}(c_o - E_o) & 1/\Delta\gamma + AC_o + 6E_o \end{pmatrix}$$

$$\hat{t}_2 = \hat{t}_3 = \hat{t}_4 = 1/F_P$$

$$\hat{t}_5 = \hat{t}_6 = 1/F_D \tag{3.7}$$

where

$$A = \frac{\Delta M}{\Delta\gamma}\,\omega^2 - 6$$

$$H = AE_o + C_o - \frac{1}{2\gamma}\left\{4I(1,1,0,E_s) + I(2,0,0,E_s)\right\}$$

$$Q = \frac{1}{\Delta\gamma} + 6E_o - C_o + \frac{1}{2\gamma}\left\{4I(1,1,0,E_s) + I(2,0,0,E_s)\right\} \tag{3.8}$$

with $E_o = -\frac{1}{2\gamma} I\,(1,0,0,E_s)$

$C_o = -\frac{1}{2\gamma} I(0,0,0,E_s)$

and

$$F_s = Q\left[1 + \Delta\gamma\left\{(AC_o + 6E_o)\right\}\right] - 6\,\Delta\gamma\;H\left[(C_o - E_o)\right] \qquad (3.9)$$

$$F_P = 1 + \frac{\Delta\gamma}{2\gamma}\left\{I\,(0,0,0,E_s) - I\,(2,0,0,E_s)\right\} \qquad (3.10)$$

and

$$F_D = 1 + \frac{\Delta\gamma}{2\gamma}\left\{I\,(0,0,0,E_s) + I\,(2,0,0,E_s) - 2I(1,1,0,E_s)\right\} \qquad (3.11)$$

Using these one can evaluate the scattering amplitude as discussed in the last chapter and the result is that the scattering amplitude $f(\underline{k},\underline{k}_o)$ can be written as the sum of three terms

$$f(\underline{k},\underline{k}_o) = f_S(\underline{k},\underline{k}_o) + f_P(\underline{k},\underline{k}_o) + f_D(\underline{k},\underline{k}_o) \qquad (3.12)$$

where the S-like wave amplitude is

$$\begin{aligned} f_S(\underline{k},\underline{k}_o) = \frac{g_S(\underline{k}_o)}{F_S}\Bigg[&\Delta M\omega^2 - 6\,\Delta\gamma + \frac{\Delta\gamma\,\Delta M\,\omega^2}{2\,\gamma}\Big\{4\;I(1,1,0,E_s) \\ &+ I(2,0,0,E_s) + I(0,0,0,E_s)\Big\} + 2\Delta\gamma\left\{1 - \frac{\Delta M\omega^2}{2\,\gamma} I(1,0,0,E_s)\right\} \\ &\times\left\{\sum_{i=1}^{3}(\cos k_i + \cos k_{oi})\right\} - \frac{2\,\Delta\gamma}{3}\left\{1 - \frac{\Delta M\omega^2}{2\,\gamma}\;I(0,0,0,E_s)\right\} \\ &\times\left\{\sum_{i=1}^{3}\cos k_i\right\}\left\{\sum_{i=1}^{3}\cos k_{oi}\right\}\Bigg] \end{aligned} \qquad (3.13)$$

The P-like wave amplitude is

$$f_P\,(\underline{k},\underline{k}_o) = -\frac{2g_S(\underline{k}_o)}{F_P}\,(\,\Delta\gamma\,)\left[\sum_{i=1}^{3}\sin k_i\;\sin k_{oi}\right] \qquad (3.14)$$

and the D-like wave amplitude is

$$f_D\,(\underline{k},\underline{k}_o) = -\frac{g_S(\underline{k}_o)}{3\,F_D}\,(\Delta\gamma)\Big[\,3(\cos k_2 - \cos k_3)(\cos k_{o2} - \cos k_{o3})$$

$$+\,(2\cos k_1 - \cos k_2 - \cos k_3)(2\cos k_{o1} - \cos k_{o2} - \cos k_{o3})\Big] \qquad (3.15)$$

When the substitutional impurity is an isotope, the P and D- wave amplitudes vanish and the S-wave amplitude remains in the form

$$f_S\,(\underline{k},\underline{k}_o) = \frac{g_S(\underline{k}_o)\;\Delta M\omega^2}{F_{Si}} \qquad (3.16)$$

where $$F_{Si} = 1 - \frac{\Delta M\,\omega^2}{2\,\gamma}\,I(0,0,0,E_s) \qquad (3.17)$$

This expression has been obtained by Callaway[8].

§ 3.3. The scattering cross section, its long wavelength limit and resonances:

Here $\underline{k}$ specifies the incident direction. As already discussed, along the symmetry axes of the crystal, $\underline{k}_o$ coincides with the direction of scattering due to the behaviour of the constant frequency surface along these directions. This facilitates the use of optical theorem to evaluate the total cross section when the phonon is incident along one of the symmetry axes. Also in the limit of long waves, this can be done for any incident direction. The scattering angle in this case is that between $\underline{k}$ and $\underline{k}_o$.

To demonstrate the use of optical theorem, we evaluate the total scattering cross section σ_T for phonons incident along (1,0,0) axis using equation (2.38). Then $\underline{k} = (k,0,0)$ and we set $\underline{k}_o = (k_o,0,0)$ to evaluate the forward scattering amplitude. $\underline{k}$ and $\underline{k}_o$ are equal in magnitude. With $\underline{k}_o = (k,0,0)$, $g_S(\underline{k}_o) = \frac{1}{4\pi\gamma}$ and the scattering cross section can be expressed in units of a^2, where a is the lattice constant, as

$$\sigma_T = \frac{1}{\gamma \sin k}\left[\frac{1}{|F_S|^2} \left(\operatorname{Im} D \operatorname{Re} F_S - \operatorname{Re} D \operatorname{Im} F_S \right) + \frac{2\Delta\gamma}{|F_P|^2} (\operatorname{Im} F_P) \sin^2 k - \frac{4\Delta\gamma}{3|F_D|^2} (\cos k - 1)^2 (\operatorname{Im} F_D) \right] \quad (3.18)$$

where

$$D = \Delta M \omega^2 - 6\,\Delta\gamma + \Delta M \omega^2 \frac{\Delta\gamma}{2\gamma} \left\{ 4\, I(1,1,0,E_s) + I(2,0,0,E_s) + I(0,0,0,E_s) \right\} + \Delta\gamma \left[4 \left\{ 1 - \frac{\Delta M \omega^2}{2\gamma} I(1,0,0,E_s) \right\} - \frac{2}{3} \left\{ 1 - \frac{\Delta M \omega^2}{2\gamma} I(0,0,0,E_s) \right\} (2+\cos k) \right] (2+\cos k) \quad (3.19)$$

and

$$\begin{aligned} \operatorname{Re} F_S = {} & 1 - \frac{\Delta M}{M}(3-E_s)\, S(0,0,0,E_s) + \frac{\Delta\gamma}{2\gamma} \left\{ 7S(0,0,0,E_s) \right. \\ & \left. + 12\, C(1,0,0,E_s) - 4\, S(1,1,0,E_s) - S(2,0,0,E_s) \right\} + \frac{\Delta\gamma}{2\gamma} \frac{\Delta M}{M} (3-E_s) \\ \times & \left[6 \left\{ C^2(1,0,0,E_s) - S^2(1,0,0,E_s) \right\} - C(0,0,0,E_s) \left\{ 4C(1,1,0,E_s) \right. \right. \\ & \left. + C(2,0,0,E_s) - C(0,0,0,E_s) \right\} + S(0,0,0,E_s) \left\{ 4S(1,1,0,E_s) \right. \\ & \left. \left. + S(2,0,0,E_s) - S(0,0,0,E_s) \right\} \right] \end{aligned} \quad (3.20)$$

$$\begin{aligned} \mathrm{Im}\, F_S = & -\frac{\Delta M}{M}(3-E_s)\, C(0,0,0,E_s) + \frac{\Delta\gamma}{2\gamma}\Big\{ 7C(0,0,0,E_s) - 12S(1,0,0,E_s) \\ & - 4C(1,1,0,E_s) - C(2,0,0,E_s)\Big\} + \frac{\Delta\gamma}{2\gamma}\,\frac{\Delta M}{M}(3-E_s) \\ & \times \Big[-12C(1,0,0,E_s)\, S(1,0,0,E_s) + C(0,0,0,E_s)\Big\{ 4S(1,1,0,E_s) \\ & + S(2,0,0,E_s) - S(0,0,0,E_s)\Big\} + S(0,0,0,E_s)\Big\{ 4C(1,1,0,E_s) \\ & + C(2,0,0,E_s) - C(0,0,0,E_s)\Big\}\Big] \end{aligned} \qquad (3.21)$$

$$\mathrm{Re}\, F_P = 1 + \frac{\Delta\gamma}{2\gamma}\Big\{ S(0,0,0,E_s) + S(2,0,0,E_s)\Big\} \qquad (3.22)$$

$$\mathrm{Im}\, F_P = \frac{\Delta\gamma}{2\gamma}\Big\{ C(0,0,0,E_s) + C(2,0,0,E_s)\Big\} \qquad (3.23)$$

$$\mathrm{Re}\, F_D = 1 + \frac{\Delta\gamma}{2\gamma}\Big\{ S(0,0,0,E_s) + 2S(1,1,0,E_s) - S(2,0,0,E_s)\Big\} \qquad (3.24)$$

$$\mathrm{Im}\, F_D = \frac{\Delta\gamma}{2\gamma}\Big\{ C(0,0,0,E_s) + 2C(1,1,0,E_s) - C(2,0,0,E_s)\Big\} \qquad (3.25)$$

Here we have used the $C(p,q,r,E_s)$ and $S(p,q,r,E_s)$ defined in Appendix I and their values have been tabulated.[28,32]

In the special case when the substitutional impurity is an isotope, $\Delta\gamma = 0$ so that $D = \Delta M \omega^2$ and $F_{Si} = 1 - \left(\frac{\Delta M \omega^2}{2\gamma}\right) I(0,0,0,E_s)$ which leads to the result

$$\sigma_{Ti} = \frac{1}{\gamma \sin k}\left(\frac{\Delta M}{2\gamma}\right)^2 \frac{\omega^4}{|F_{Si}|^2}\, \mathrm{Im}(I\,(0,0,0,E_s)) \qquad (3.26)$$

We define $$\omega_{oS}^2 = \frac{2\gamma}{M} \qquad (3.27)$$

and in the limit of long waves

$$\frac{1}{2\gamma}\,\mathrm{Im}\Big\{ I(0,0,0,E_s)\Big\} = \frac{1}{2\gamma}\, C(0,0,0,E_s) = \frac{k}{4\pi\gamma} = \frac{k}{4\pi M \omega_{oS}^2} \qquad (3.28)$$

and then with $\sin k \rightarrow k$, equation (3.26) yields

$$\sigma_T = \frac{1}{\pi} \left(\frac{\Delta M}{M} \right)^2 \frac{\omega^4}{\omega_{oS}^4} \frac{1}{|F_{Si}|^2} \text{ in units of } a^2. \quad (3.29)$$

This is exactly the expression obtained by Callaway[9]. The scattering is purely S-wave type.

The long wavelength limit of σ_T of equation (3.18) is given by

$$\sigma_T = \frac{1}{\gamma k} \Big[\frac{1}{|F_S|^2} \left\{ \text{Im } D \text{ Re } F_S - \text{Re } D \text{ Im } F_S \right\} + \frac{2\Delta\gamma}{|F_P|^2} k^2 (\text{Im } F_P) + \frac{\Delta\gamma}{3|F_D|^2} k^4 (-\text{Im } F_D) \Big] \quad (3.30)$$

where the quantity D now becomes

$$D = \Delta M \omega^2 - (k^4/6)\Delta\gamma + \frac{\Delta\gamma . \Delta M \omega^2}{2\gamma} \left\{ 4I(1,1,0,E_s) + I(2,0,0,E_s) + 7I(0,0,0,E_s) - 12I(1,0,0,E_s) \right\} + \frac{\Delta\gamma \, \Delta M \omega^2 k^2}{\gamma} \left\{ I(1,0,0,E_s) - I(0,0,0,E_s) \right\} \quad (3.31)$$

where $I(p,q,r,E_s)$ are to be evaluated in the limit of long waves. Retaining terms upto the order of ω^4, the D-wave amplitude does not contribute because it is of the order of ω^6 and hence

$$\sigma_T = \frac{1}{\pi} \Big[\left(\frac{\Delta M}{M} \right)^2 \frac{1}{|F_S|^2} \left(1 + b \frac{\Delta\gamma}{\gamma} \right)^2 + \frac{4}{3} \left(\frac{\Delta\gamma}{\gamma} \right)^2 \frac{1}{|F_P|^2} \Big] \left(\frac{\omega}{\omega_{oS}} \right)^4 \quad (3.32)$$

in units of a^2, where the constant $b \simeq 1.14$. This result shows that in the long wavelength (low frequency) limit, the scattering cross section is proportional to ω^4 showing Rayleigh type of scattering, provided that there is no resonance which is seen by examining Re F_S and Re F_P. The S-wave part of the cross section is affected by both ΔM and $\Delta\gamma$ whereas the P-wave part depends only upon $\Delta\gamma$.

It is worth while to point out that the number of partial waves contributing to the total scattering cross-section depends strongly upon the direction of incidence. This is discussed in some detail in the next chapter. For example if we evaluate the scattering cross section for the (1,1,1) direction of incidence the D-wave part will not contribute to an expression like that given in equation (3.18).

A resonance in the scattering cross section will occur for that value of the frequency at which any of the quantities ReF_S, Re F_P or Re F_D vanishes and the width $\Gamma_\omega = \frac{\text{Im } F}{(\text{Re } F)'}$ is small and positive. The real and imaginary parts of F_S, F_P and F_D are given by equations (3.20) to (3.25). One can study the resonances by taking given values of $\frac{\Delta M}{M}$ and $\frac{\Delta\gamma}{\gamma}$ and examining the criteria for resonance. The figures 1 and 2 give the results of such a study. In these the value of the parameter E_s, defined in Appendix I is found at resonance for given values of $\frac{\Delta M}{M}$ and $\frac{\Delta\gamma}{\gamma}$. We find that the P and D resonances depend upon $\Delta\gamma$ only. For sufficient decrease in force constant the P and D resonances appear at the low frequency side of the band. If this is increased the resonances appear towards the high frequency side of the band. Indeed in figure 2 if one changes the sign of $\Delta\gamma/\gamma$ the corresponding E_{SR} simply reverses the sign having its magnitude intact.

The S-wave resonances depend upon ΔM as well as $\Delta\gamma$. For a large increase in mass, resonances appear towards the low frequency

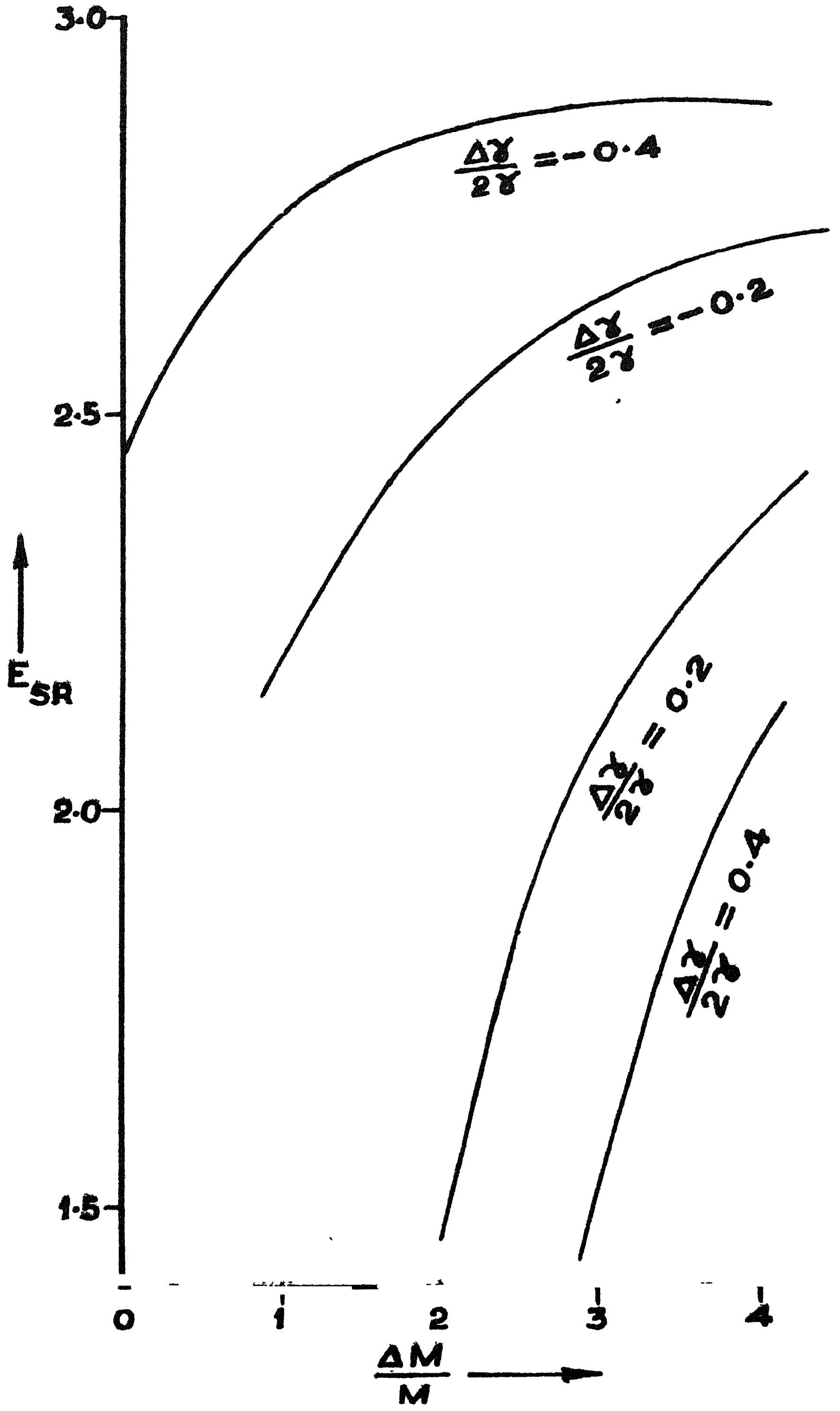


Figure 1: E_{sr} is plotted against the parameter $\frac{\Delta M}{M}$ for the S-wave part for the simple cubic latice.

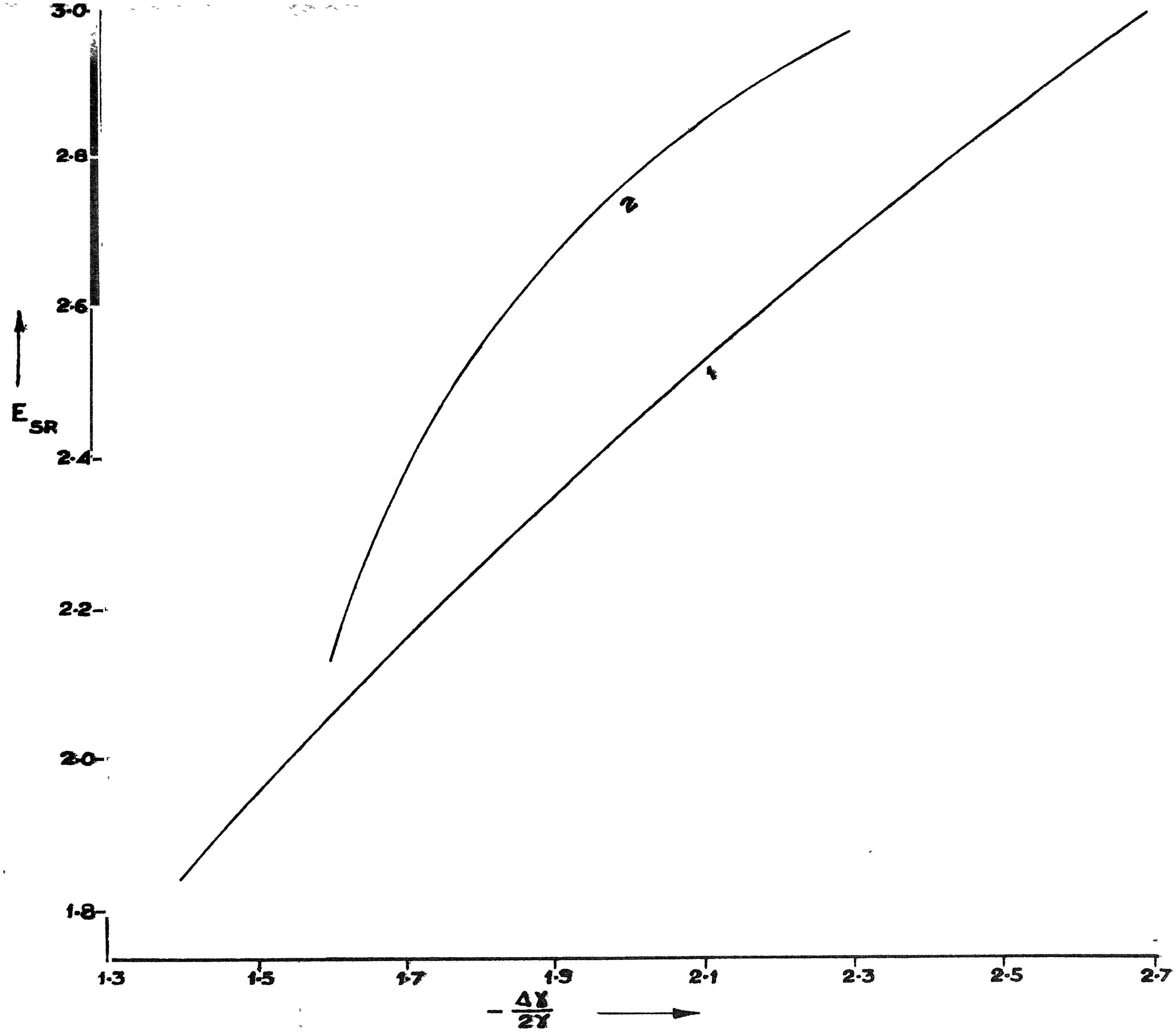


Figure 2. E plotted against the parameter $\Delta\gamma$

(large positive E_S) side of the band, no matter what the change in force constant is. On the other hand, for small changes in mass, the change in force constant plays a dominant role in determining the resonances. At resonances, the scattering cross section does not have a ω^4 dependence in the limit of long waves. Since the real parts of F_S and F_P become zero and the imaginary parts of F_S and F_P are proportional to $\left(\frac{\omega}{\omega_{oS}}\right)^3$, then equation (3.30) for σ_T shows that it is proportional to $\left(\frac{\omega}{\omega_{oS}}\right)^{-2}$ at resonance. Further the width of the resonance is proportional to $\left(\frac{\omega}{\omega_{oS}}\right)^3$. Thus the value of σ_T at resonance becomes large by a factor $\left(\frac{\omega}{\omega_{oS}}\right)^{-6}$ with small ω. Using the expressions given by equations (3.20), (3.22) and (3.24), one can study the localized modes of S,P and D symmetries.

§ 3.4 Phonon scattering and the mean free path:

We evaluate the mean free path of phonons in the limit of long waves by using equation (2.48). The differential scattering cross section $\sigma_D(\theta)$ in this limit is simply the square of the scattering amplitude which is given by

$$f(\theta) = \left[\frac{1}{2\pi}\left(\frac{\Delta M}{M}\right)\left(1 + b\,\frac{\Delta\gamma}{\gamma}\right)\frac{1}{F_S} - \frac{1}{\pi}\left(\frac{\Delta\gamma}{\gamma}\right)\left(\frac{1}{F_P}\right)\cos\theta \right] \times \left(\frac{\omega}{\omega_{oS}}\right)^2 \qquad (3.33)$$

with $b \simeq 1.14$ and θ is the scattering angle.

Then

$$\frac{1}{\Lambda(\omega)} = 2\pi N_c \int_0^{\pi} \left| f(\theta) \right|^2 (1-\cos\theta)\sin\theta \, d\theta$$

$$= \frac{4\,N_c a^2}{\pi}\left(\frac{\omega}{\omega_{oS}}\right)^4\left[\frac{1}{4}\left(\frac{\Delta_M}{M}\right)^2\left(1+b\,\frac{\Delta\gamma}{\gamma}\right)^2\frac{1}{|F_S|^2}+\frac{1}{3}\left(\frac{\Delta\gamma}{\gamma}\right)^2\frac{1}{|F_P|^2}\right.$$

$$\left.+\frac{1}{6}\left(\frac{\Delta\gamma}{\gamma}\right)\left(\frac{\Delta_M}{M}\right)\left(1+b\,\frac{\Delta\gamma}{\gamma}\right)\left(\frac{1}{F_S^{*}F_P}+\frac{1}{F_S F_P^{*}}\right)\right] \qquad (3.34)$$

The last term on the right hand side is the interesting term showing the interference between terms of opposite 'parities'. Here 'parity' signifies the behavior under inversion at the centre of inversion. The S-type of term does not change sign under inversion and it is the so called 'gerade' term and the P-type is 'ungerade'.

At resonance the ω^4 proportionality of $\Lambda^{-1}(\omega)$ does not hold and the dominant term can be shown to be proportional to ω^{-2} as in the case of σ_T.

Thus the simple model considered here shows the important features of the scattering of phonons except the question of polarization which is discussed in chapter V. The long wave length Rayleigh type of scattering and the modifications at resonances are explicitly obtained here. The directional dependence of the scattering cross section, the interference of terms of different symmetries in the mean free path expression are the other important features of the process and these are further elaborated in chapters IV and V. In the following section we consider a model of diatomic simple cubic lattice to demonstrate the ease with which the results for the mono-atomic lattices can be carried over to the study of diatomic lattice. In fact this feature adds to the usefulness of the results for mono-atomic lattices.

§ 3.5 Diatomic Simple cubic lattice:-

Let a diatomic simple cubic lattice be considered whose atoms of type I have mass M_1 each and those of type II have mass M_2 each. The central and non-central harmonic force constant between nearest neighbours is denoted by γ. One can write down the equations of motion and perform the so called M^* transformation used by Montroll and Potts[4-5] so that the equations of motion for the diatomic lattice becomes identical to those of monoatomic lattice with $M^* \omega^2$ in place of $M \omega^2$ where,

$$M^* \omega^2 = 6\gamma + \sqrt{(M_1 \omega^2 - 6\gamma)(M_2 \omega^2 - 6\gamma)} \qquad (3.35)$$

Then the dispersion becomes

$$M^* \omega^2(\underline{k}) = 6\gamma - 2\gamma \sum_i \cos k_i \qquad (3.36)$$

and this leads to

$$\sqrt{(M_1 \omega^2(\underline{k}) - 6\gamma)(M_2 \omega^2(\underline{k}) - 6\gamma)} = -2\gamma \sum_i \cos k_i \qquad (3.37)$$

Solving this equation for $\omega^2(\underline{k})$ one gets the optical and acoustic branches as,

$$\omega^2_{op}(\underline{k}) = 3\gamma \left(\frac{1}{M_1} + \frac{1}{M_2}\right)\left[1 + \sqrt{1 - \frac{4\left(1 - \frac{1}{3}\sum_i \cos k_i\right)}{M_1 M_2 \left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2}}\,\right] \qquad (3.38a)$$

and

$$\omega^2_{ac}(\underline{k}) = 3\gamma \left(\frac{1}{M_1} + \frac{1}{M_2}\right)\left[1 - \sqrt{1 - \frac{4\left(1 - \frac{1}{3}\sum_i \cos k_i\right)}{M_1 M_2 \left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2}}\,\right] \qquad (3.38b)$$

The maximum frequency in the optical band is $\omega^2_{opM} = 6\gamma\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$ and the minimum frequency in the acoustic band is

$\omega^2_{acm} = 0$. The minimum in the optical band ω^2_{opm} and the maximum in the acoustic band ω^2_{acM} depend upon the relative magnitude of M_1 and M_2 . For $M_1 > M_2$, $\omega^2_{opm} = \frac{6\gamma}{M_2}$ and $\omega^2_{acM} = \frac{6\gamma}{M_1}$ whereas for $M_2 > M_1$, $\omega^2_{opm} = \frac{6\gamma}{M_1}$ and $\omega^2_{acM} = \frac{6\gamma}{M_2}$. The gap between the two bands is of magnitude $6\gamma \left| (1/M_1 - 1/M_2) \right|$.

In analogy with the monoatomic case the Green function integral becomes ,

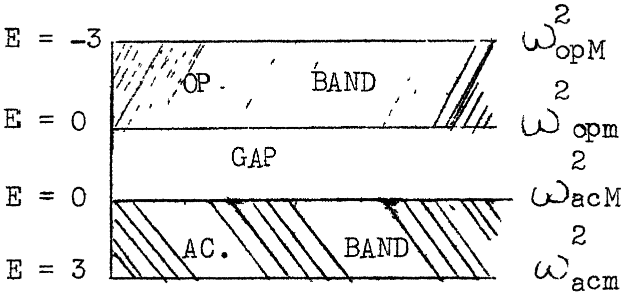
$$G(\omega^2, l, m, n) = -1/N \sum_{\underline{k}} \frac{\exp\{i(k_1 l + k_2 m + k_3 n)\}}{M^* \omega^2(\underline{k}) - M^* \omega^2 - i\epsilon}$$

$$= -\frac{1}{2\gamma N} \sum_{\underline{k}} \frac{\exp\{i(k_1 l + k_2 m + k_3 n)\}}{E - \sum_i \cos k_i} \qquad (3.39)$$

where
$$E = -\frac{1}{2\gamma} \sqrt{(M_1 \omega^2 - 6\gamma)(M_2 \omega^2 - 6\gamma)} \qquad (3.40)$$

$$= -3 \sqrt{\left(\frac{\omega^2}{\omega^2_{acM}} - 1\right)\left(\frac{\omega^2}{\omega^2_{opm}} - 1\right)} \qquad (3.41)$$

It may be noted that at each step one can check the results with that for the monoatomic lattice by setting $M_1 = M_2$. The quantity E goes over to $E_s = 3 - \frac{\omega^2}{\omega^2_{os}}$ for $M_1 = M_2$. In terms of the E defined above, $3 \geqslant E \geqslant 0$ defines the acoustic band and $0 \geqslant E \geqslant -3$ defines the optical band. Within the gap, E has an imaginary value. These have been discussed in detail by Mitani and Takeno [43].



Thus taking appropriate values of E one can consider the scattering of phonons in both the acoustic and optical bands. Optical phonons do not contribute to the low temperature thermal conductivity, but it is interesting to consider the scattering of optical phonons from the substitutional impurity.

Consider a substitutional impurity put at a site of an atom of type I which may be taken to be the origin of the coordinate system. Let its mass be $M_1 + \Delta M$ and the force constant be $\gamma + \Delta\gamma$. The elements of the perturbation matrix after the M^* transformation get modified into the following,

$$p(\underline{0},\underline{0}) = \xi\,(M\omega^2 - 6\gamma), \quad p(\underline{0}, \underline{R}_n) = p(\underline{R}_n, \underline{0}) = \Delta\gamma .$$

$$p(\underline{R}_n, \underline{R}_n) = -\frac{\Delta\gamma}{\xi} .$$

Following the method described in this chapter (after performing the M^* transformation) one gets the following resonance denominators also obtained by Mitani and Takeno[43].

$$F_S = 1 + \frac{\Delta\gamma}{\gamma} - \left(\frac{\Delta\gamma}{\gamma} - \frac{\Delta M}{M_1} \right) M_1 \omega^2 \xi\, G(\omega^2,0,0,0) + \left(\frac{\Delta\gamma}{\gamma} \right) \left(1 + \frac{\Delta M}{M_1} \right) M_1 \omega^2 G(\omega^2,1,0,0) \qquad (3.42)$$

$$F_P = 1 - \left(\frac{\Delta\gamma}{\xi}\right) \left\{ G(\omega^2,0,0,0) - G(\omega^2,2,0,0) \right\} \qquad (3.43)$$

and
$$F_D = 1 - \left(\frac{\Delta\gamma}{\xi}\right) \left\{ G(\omega^2,0,0,0) + G(\omega^2,2,0,0) \right\} - 2G(\omega^2,1,1,0) \qquad (3.44)$$

where
$$\xi = \sqrt{(M_2\omega^2 - 6\gamma) / (M_1\omega^2 - 6\gamma)} \qquad (3.45)$$

Within the bands, the parameter E is real and the Green functions occuring above can be written in terms of I (p,q,r, E) as,

$$C\,(\omega^{2},\ p,q,r,) = -\frac{1}{2\gamma}\ I\,(p,q,r,E) \qquad (3.46)$$

which in turn can be written in terms of the tabulated functions C (p,q,r,E) and S (p,q,r,E) . Here ω^{2} is related to E by the relations,

(i) Optical band,

$$\omega^{2} = \tfrac{1}{2}\left[(\omega^{2}_{opm} + \omega^{2}_{acM}) + \sqrt{(\omega^{2}_{opm} - \omega^{2}_{acM})^{2} + 4\,(E^{2}/9)\,\omega^{2}_{opm}\,\omega^{2}_{acM}}\right] \qquad (3.47)$$

and (ii) Acoustic Band,

$$\omega^{2} = \tfrac{1}{2}\left[(\omega^{2}_{opm} + \omega^{2}_{acM}) - \sqrt{(\omega^{2}_{opm} - \omega^{2}_{acM})^{2} + 4\,(E^{2}/9)\,\omega^{2}_{opm}\,\omega^{2}_{acM}}\right] \qquad (3.48)$$

Using the above expressions for the resonance denominators Mitani and Takeno[43] have investigated the localized modes both above the top of the optical band and within the gap between the acoustic and optical bands. We have investigated the resonances in the acoustic and optical bands and the results are given in the figures 3 to 6 for the cases; (i) $M_1 > M_2$, $p = M_2/M_1 = 2$ and (ii) $M_2 > M_1$, $p = M_2/M_1 = \frac{1}{2}$. These are the same as those used by Mitani and Takeno[43] for investigating the localized modes.

The change in mass does not affect the resonances in P and D like waves. Resonances only in the optical band are shown for these waves. The result is very similar to that of the monoatomic lattice case and as the force constant increases, the resonance frequency moves to-wards the high frequency edge of the band.

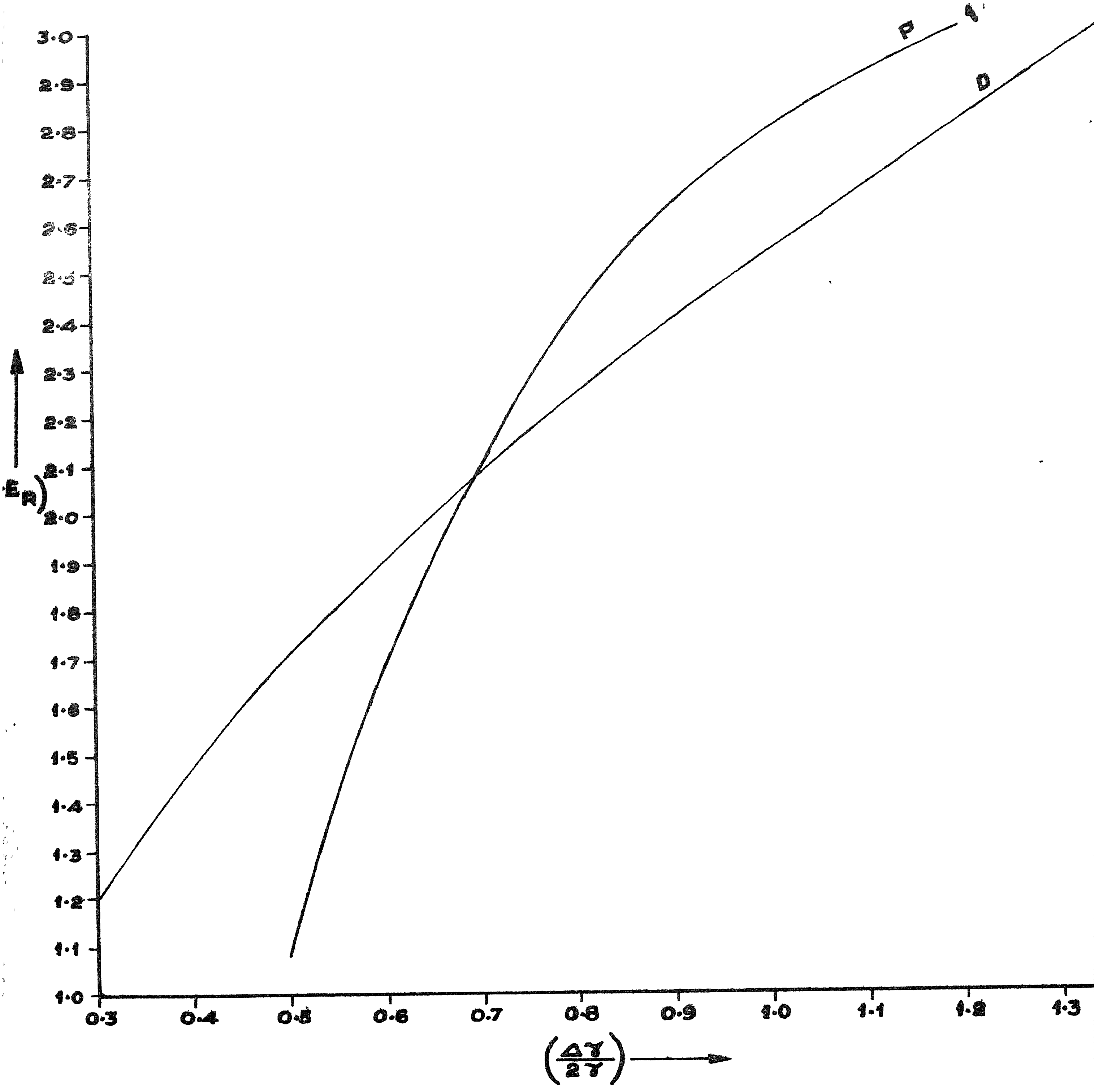


Figure 3. P and D-wave resonances for $M_1 > M_2$ and $p = M_2/M_1 = \frac{1}{2}$ in Optical band for diatomic simple cubic lattice.

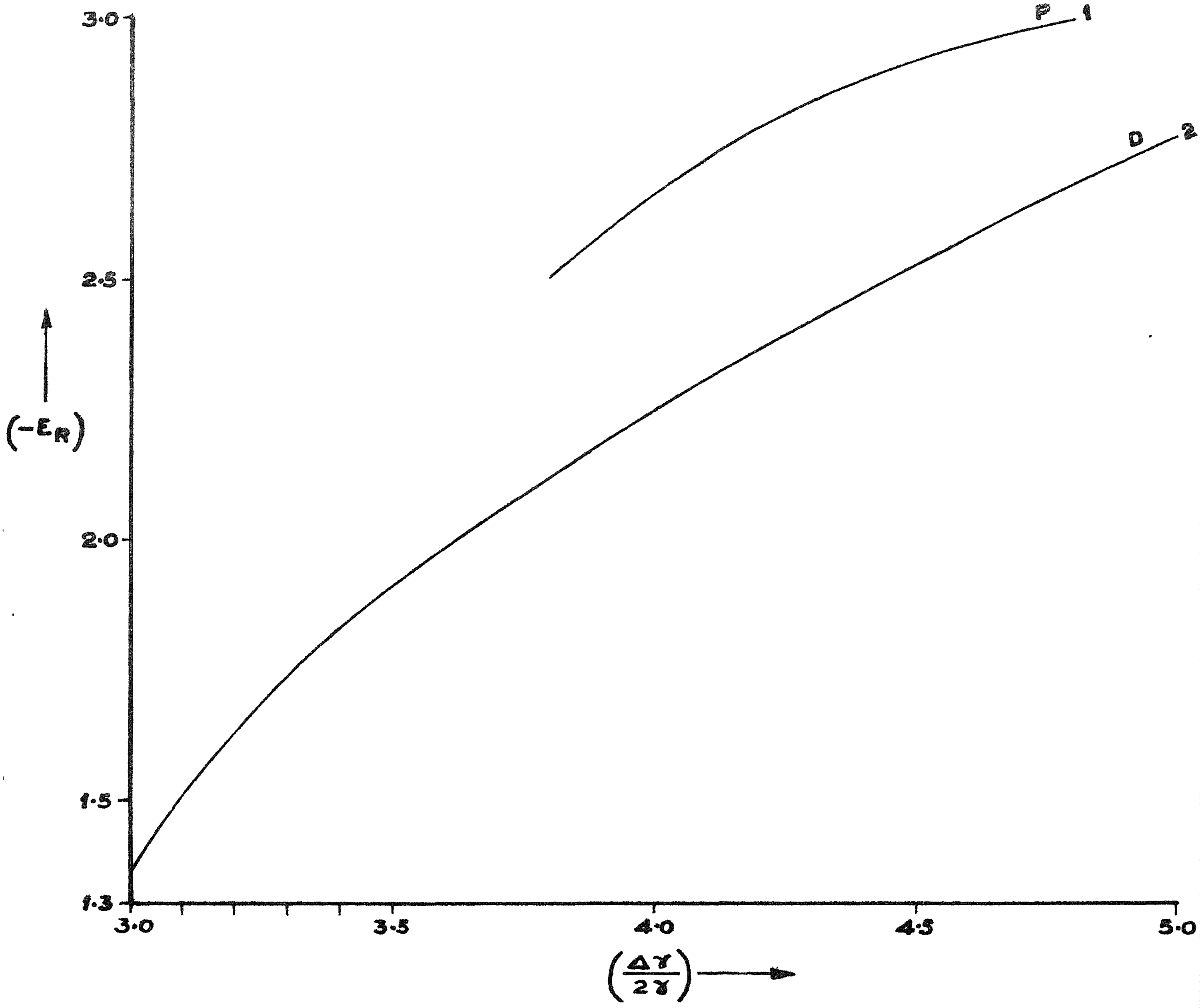


Figure 4: P and D-wave resonances for $M_2 > M_1$ and $p = M_2/M_1 = 2$ in the Optical band of diatomic simple cubic lattice.

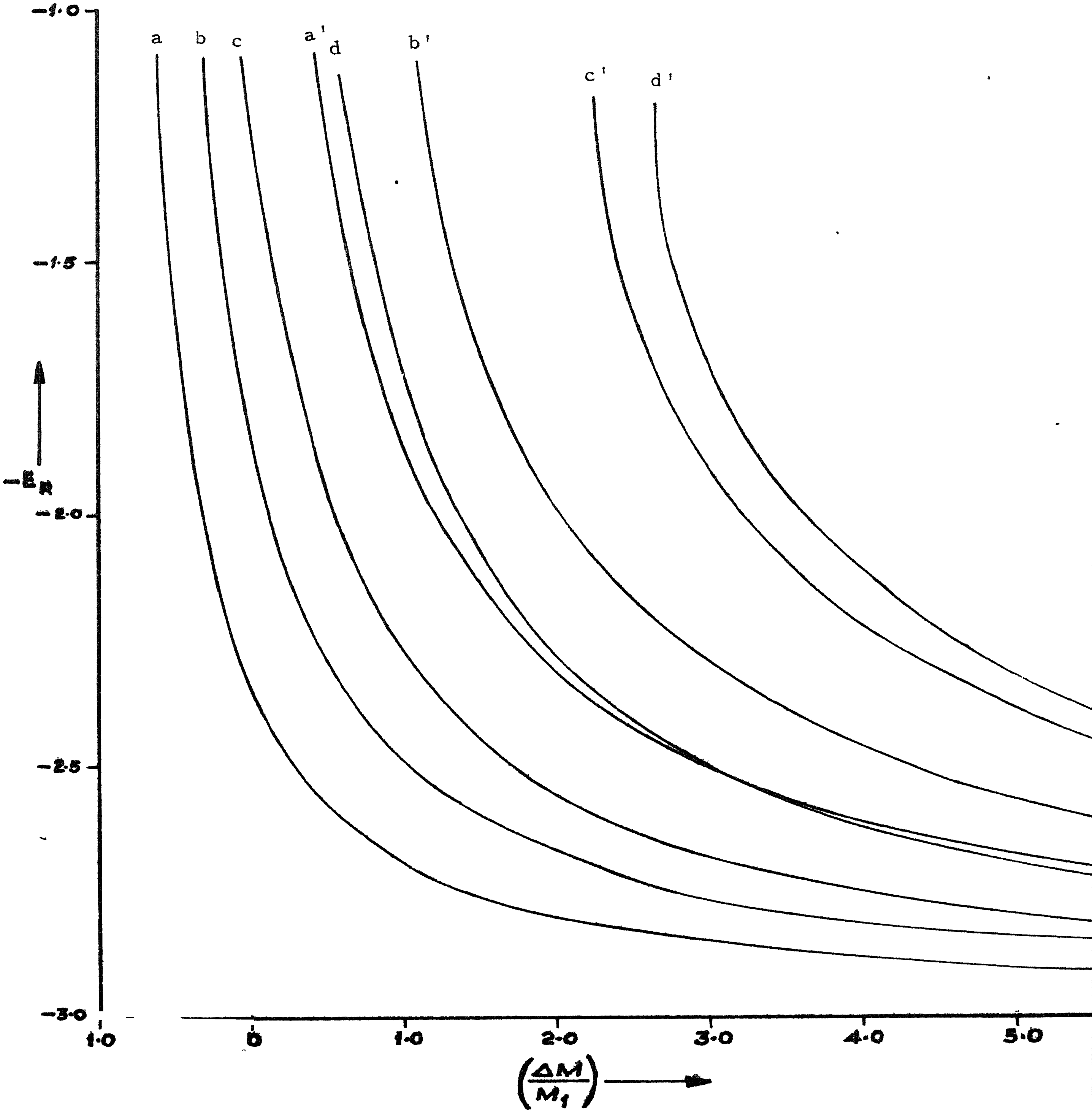


Figure 5: Typical S-wave resonances in Acoustic Band of diatomic simple cubic lattice. Curves a, b, c, and d are for $M_1 > M_2$, p=1/2 with $\Delta\gamma/\gamma$ =-.7, -.5, -.3, +.1 respectively and curves a', b', c' and d' are for $M_2 > M_1$, p=2, with $\Delta\gamma/\gamma$ =-.5, -.3, 0 and +.1 respectively.

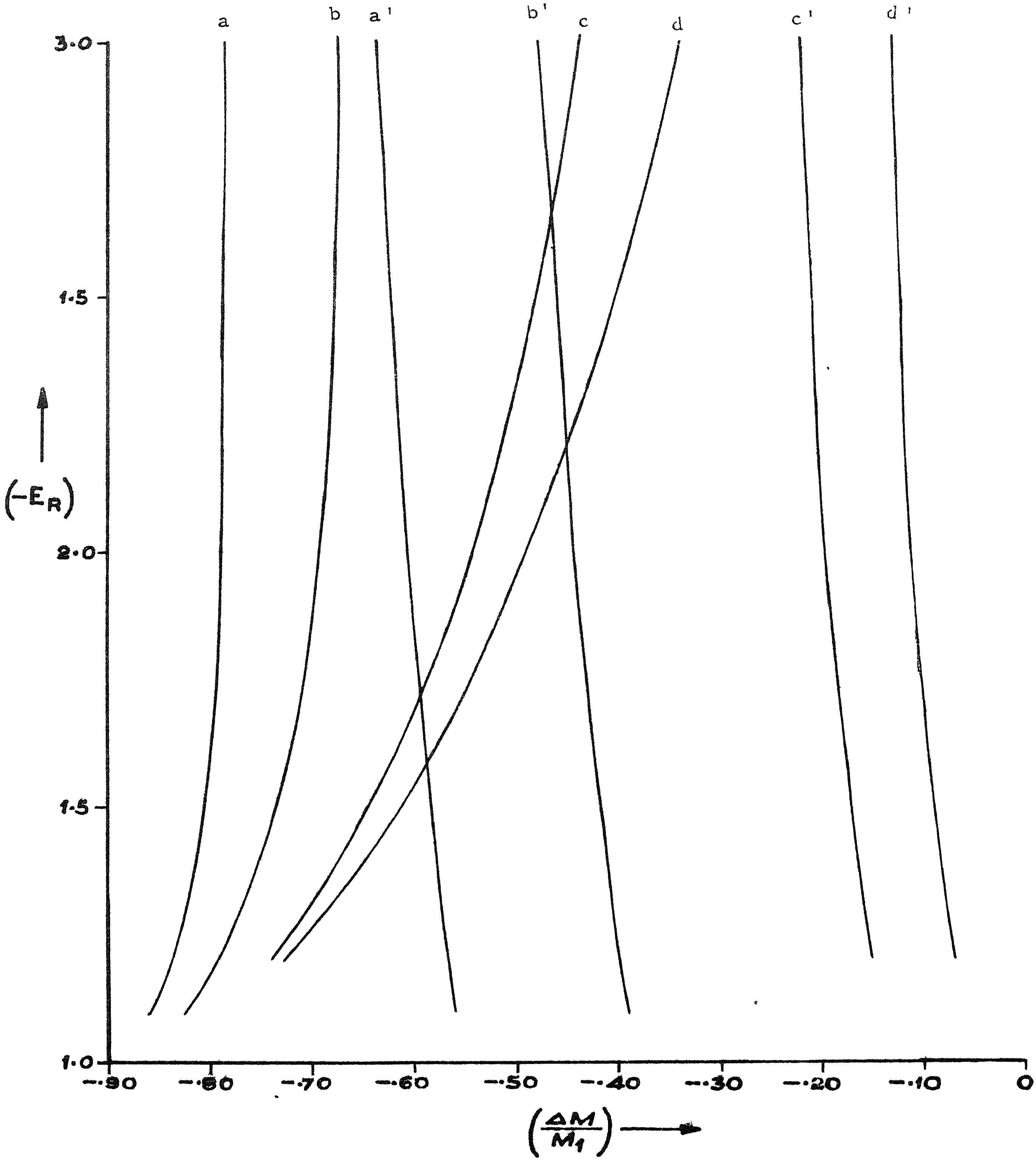


Figure 6. Typical S-wave Resonances in the Optical band of a diatomic simple cubic lattice. **lattice.** Curves a, b, c and d are for $M_1 > M_2$, p= 1/2 with $\Delta\gamma/\gamma$=-.5, -.3 0 and +.1 respectively and curves a', b', c' and d' are for $M_2 > M_1$, p=2, with $\Delta\gamma/\gamma$=-.5, -.3, 0 and +.1 respectively.

In all the figures E_R denotes the value of E at resonance. For the case $M_1 > M_2$ which implies that the substitutional impurity has been put at the site of an atom of mass M_1 (heavier mass), comparatively low values of increase in force constant produce P and D wave resonances in the optical band. For higher values of increase in the force constant one gets these resonances if an atom of mass M_2 is substituted by the impurity.

The S - wave resonances are interesting. In the acoustic band one gets the usual result that as the increase in mass becomes large, one gets low frequency resonances, no matter what the value of the change in force constant is. This remains true for both the cases of (i) $M_1 > M_2$ and (ii) $M_2 > M_1$. But in the optical band one gets different behaviors for these two cases. When the site of the heavier atom is substituted ($M_1 > M_2$) , one gets resonances for a decrease in mass and the smaller masses give rise to resonances nearer to the bottom of the optical band. When the site of the lighter atom is substituted, one gets resonances for which the smaller masses give rise to resonances near the top of the optical band. It is interesting to note that from E = 0 to E = - 1 large decrease in force constant is required to get resonances (not shown in the figure). This can perhaps be attributed to the behavior of the density of phonon states in this interval.

From the above analysis it becomes clear that while in the monoatomic case, only heavy masses can produces resonances and light masses give rise to localized modes, in the diatomic lattice light masses can produce localized modes above the optical band and resonances in the optical band. In addition one can get localized modes in the gap. The present analysis,along with that of Mitani and Takeno[43] leads to a rather complete analysis of the problem for diatomic simple cubic lattice.

CHAPTER IV

BODY CENTRED CUBIC AND FACE CENTRED CUBIC LATTICES

§ 4.1 The Model

In this chapter the results of a study of the problem of scattering of phonons from a substitutional impurity in a simplified model of face centred cubic and body centred cubic lattices are presented. The method of analysis is the same as that presented in chapter II. The displacements of the atoms in the lattice are assumed to be scalar parameters which depend upon lattice sites. This is not realistic for lattice dynamics as there would be no polarisation of phonons in this model. However, some essential features of the process of scattering are brought out even in this model and one can get a qualitative insight into the problem of scattering in more realistic lattices. As shown in chapter V, the results of the present chapter can be obtained by a suitable choice of force constants in a realistic model. The present analysis is, however, completely applicable in the problem of scattering of spin waves or band electrons from substitutional impurities.

In the two lattice models considered here each atom has mass M and nearest neighbour harmonic force constant γ , except for the impurity atom which has mass $M + \Delta M$ and is coupled to its nearest neighbours through a force constant $\gamma + \Delta\gamma$. The impurity is taken to be at the origin and the lattice vectors $\underline{R}$ have Cartesian components[44],

$$\underline{R}_B = (\ell + m/2)a\,\underline{e}_1 + (m/2)a\,\underline{e}_2 + (n + m/2)a\,\underline{e}_3 \qquad (4.1a)$$

and

$$\underline{R}_F = \tfrac{1}{2}(\ell + n)a\,\underline{e}_1 + \tfrac{1}{2}(\ell + m)a\,\underline{e}_2 + \tfrac{1}{2}(m + n)a\,\underline{e}_3 . \qquad (4.1b)$$

here a is the length of the side of the unit cell and $\underline{e}_i$ are the unit vectors along the Cartesian axes, and ℓ, m, and n are integers. The total number of atoms is N. The subscripts B and F refer to Body Centred Cubic and face centred cubic lattices respectively.

The frequencies (squared) are given by,

$$\omega_B^2(\underline{k}) = \omega_{OB}^2 \left(1 - \cos\frac{k_1}{2}\ \cos\frac{k_2}{2}\ \cos\frac{k_3}{2}\right), \quad (4.2a)$$

and

$$\omega_F^2(\underline{k}) = \omega_{OF}^2 \left(3 - \cos\frac{k_1}{2}\cos\frac{k_2}{2} - \cos\frac{k_2}{2}\cos\frac{k_3}{2} - \cos\frac{k_3}{2}\cos\frac{k_1}{2}\right), \quad (4.2b)$$

where $\omega_{OB}^2 = 8\,\gamma/M$, $\omega_{OF}^2 = 4\,\gamma/M$, and k_i are the Cartesian components of the wave number $\underline{k}$. These can be obtained by writing the equations of motion in the form of equation (2.1) with the components of $\hat{A}_{B,F}$ given by ,

$$\begin{aligned} A_B(\ell mn, \ell' m' n') = \gamma \Big[& 8\,\delta_{\ell',\ell}\,\delta_{m',m}\,\delta_{n',n} - \delta_{\ell',\ell}\,\delta_{n',n}(\delta_{m',m+1} + \delta_{m',m-1}) \\ & - \delta_{n',n}(\delta_{\ell',\ell+1}\,\delta_{m',m-1} + \delta_{\ell',\ell-1}\,\delta_{m',m+1}) \\ & - \delta_{\ell',\ell}(\delta_{m',m-1}\,\delta_{n',n+1} + \delta_{m',m+1}\,\delta_{n',n-1}) \\ & - (\delta_{\ell',\ell+1}\,\delta_{m',m-1}\,\delta_{n',n+1} \\ & \quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\,\delta_{n',n-1}) \Big] \end{aligned} \qquad (4.3a)$$

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$$A_F(lmn,\ l'm'n') = \sqrt{}\Big[12\,\delta_{l',l}\,\delta_{m',m}\,\delta_{n',n} - \delta_{l',l}\,\delta_{m',m}(\delta_{n',n+1} + \delta_{n',n-1})$$

$$-\delta_{l',l}\,\delta_{n',n}(\delta_{m',m+1} + \delta_{m',m-1}) - \delta_{m',m}\,\delta_{n',n}(\delta_{l',l+1} + \delta_{l',l-1})$$

$$-\delta_{l',l}(\delta_{m',m+1}\,\delta_{n',n-1} + \delta_{m',m-1}\,\delta_{n',n+1}) - \delta_{m',m}(\delta_{l',l+1}\,\delta_{n',n-1}$$

$$+\delta_{l',l-1}\,\delta_{n',n+1})$$

$$-\delta_{n',n}(\delta_{l',l+1}\,\delta_{m',m-1} + \delta_{l',l-1}\,\delta_{m',m+1})\Big] \qquad (4.3\ b)$$

The perturbation matrix $\hat{P}$ of equation (2.5) for these cases has non-vanishing elements only when the indices refer to the impurity site and its nearest neighbours. We shall denote the nearest neighbour vectors by $\underline{R}_n$. The non-vanishing elements for the two lattices are,

$$P(\underline{0},\underline{0}) = \Delta M\,\omega^2 - (Z_{B,F})\,\Delta\gamma, \quad P(\underline{R}_n,\underline{R}_n) = -\Delta\gamma,$$

$$P(\underline{0},\underline{R}_n) = P(\underline{R}_n,\underline{0}) = \Delta\gamma, \qquad (4.4)$$

where $Z_B = 8$, and $Z_F = 12$.

The unperturbed normal modes are given by,

$$U^{(0)}_{\underline{k}}(\underline{R}) = N^{-\frac{1}{2}} \exp(i\,\underline{k}.\underline{R}/a) \qquad (4.5)$$

The elements of the Green function matrix, along with their low frequency expansions are given in Appendix I.

§ 4.2 The partial wave analysis

Here the point group of the lattice is the cubic group O_h. The representation of O_h generated by the displacements of the affected lattice sites reduces, in the usual notation[42] to,

$$\Gamma_B = 2\,A_{1g} + F_{1u} + F_{2g} + A_{2u} \quad , \tag{4.6 a}$$

and

$$\Gamma_F = 2\,A_{1g} + F_{1u} + E_g + F_{2g} + F_{2u} \quad . \tag{4.6 b}$$

One can use the method of projection operators to obtain the symmetry vectors which constitute the columns of $\hat{V}$ matrix as described in Appendix III, where $\hat{V}_B$ and $\hat{V}_F$ are found explicitly.

The indices of rows and columns of the $\hat{V}$ matrices as specified in Appendix III for $\hat{V}_B$ and $\hat{V}_F$ are used similarly to write the matrices $\hat{P}_B$, $\hat{P}_F$ and $\hat{G}_F$ in their explicit forms.

The inverse block matrices $\hat{t}_i$ occuring in equation (2.28) are as follows. For the body centred cubic lattice.

$$\hat{t}_{1B} = \frac{1}{F_{SB}} \begin{bmatrix} 1 + \Delta M\omega^2\, g_{1B} - m_B & -8^{\frac{1}{2}} m_B \\ -8^{\frac{1}{2}}\Delta\gamma(g_{0B} - g_{1B}) & 1 + A_B\, g_{0B} + 8\,\Delta\gamma\, g_{1B} \end{bmatrix} ,$$

$$\hat{t}_{2B} = \hat{t}_{3B} = \hat{t}_{4B} = \frac{1}{F_{PB}} \; , \; \hat{t}_{5B} = \hat{t}_{6B} = \hat{t}_{7B} = \frac{1}{F_{DB}} \; ,$$

and
$$\hat{t}_{8B} = \frac{1}{F_{FB}} \quad . \tag{4.7}$$

Here,

$$A_B = \Delta M\,\omega^2 - 8\,\Delta\gamma \; , \tag{4.8}$$

$$m_B = A_B\, g_{1B} + \Delta\gamma(3\,g_{2B} + 3g_{3B} + g_{0B} + g_{4B}) \; , \tag{4.9}$$

$$F_{SB} = (1 + \Delta M\,\omega^2 g_{1B} - m_B)\,(1 + A_B\, g_{0B} + 8\,\Delta\gamma\, g_{1B}) - 8\, m_B\,\Delta\gamma\,(g_{0B} - g_{1B}) \; , \tag{4.10}$$

$$F_{PB} = 1 - \Delta\gamma(g_{0B} + g_{2B} - g_{3B} - g_{4B}) \ , \qquad (4.11)$$

$$F_{DB} = 1 - \Delta\gamma(g_{0B} - g_{2B} - g_{3B} + g_{4B}) \ , \qquad (4.12)$$

and,

$$F_{FB} = 1 - \Delta\gamma(g_{0B} - 3g_{2B} + 3g_{3B} - g_{4B}) \ . \qquad (4.13)$$

The notation for the Green functions g_{iB} is described in Appendix I. With these, the scattering amplitude is,

$$f_B(\underline{k}, \underline{k}_o) = f_{SB}(\underline{k}, \underline{k}_o) + f_{PB}(\underline{k}, \underline{k}_o) + f_{DB}(\underline{k}, \underline{k}_o) + f_{FB}(\underline{k}, \underline{k}_o) \ , \qquad (4.14)$$

where,

$$f_{SB}(\underline{k}, \underline{k}_o) = \frac{g_B(\underline{k}_o)}{F_{SB}} \Big[(1 + \Delta M \omega^2 g_{1B} - m_B)(A_B + 8\Delta\gamma C_1C_2C_3) - 8\Delta\gamma m_B(1 - C_1C_2C_3) + 8\, C_{o1}C_{o2}C_{o3} \cdot \Delta\gamma \times \Big\{ (1 - C_1C_2C_3)(1 + A_B g_{0B} + 8\Delta\gamma g_{1B}) - (g_{0B} - g_{1B})(A_B + 8\Delta\gamma C_1C_2C_3) \Big\} \Big] \ , \qquad (4.15)$$

$$f_{PB}(\underline{k}, \underline{k}_o) = -\frac{8}{F_{PB}} g_B(\underline{k}_o) \Big[S_1C_2C_3S_{o1}C_{o2}C_{o3} + S_2C_3C_1S_{o2}C_{o3}C_{o1} + S_3C_1C_2S_{o3}C_{o1}C_{o2} \Big] \qquad (4.16)$$

$$f_{DB}(\underline{k}, \underline{k}_o) = \frac{8}{F_{DB}} g_B(\underline{k}_o) \Big[C_1S_2S_3C_{o1}S_{o2}S_{o3} + C_2S_3S_1C_{o2}S_{o3}S_{o1} + C_3S_1S_2C_{o3}S_{o1}S_{o2} \Big] \ , \qquad (4.17)$$

and,

$$f_{FB}(\underline{k}, \underline{k}_o) = -\frac{8}{F_{FB}} g_B(\underline{k}_o) S_1S_2S_3S_{o1}S_{o2}S_{o3} \ . \qquad (4.18)$$

Here $C_i = \cos (k_i/2)$, $S_i = \sin (k_i/2)$, $C_{oi} = \cos (k_{oi}/2)$ and $S_{oi} = \sin (k_{oi}/2)$. The expression for $g_B(\underline{k}_o)$ is given in Appendix II.

Similarly, for the face centred cubic lattice one obtains,

$$\hat{t}_{1F} = \frac{1}{F_{SF}} \begin{pmatrix} 1 + \Delta M \omega^2 g_{1F} - m_F & -12^{\frac{1}{2}} m_F \\ -12^{\frac{1}{2}} \Delta\gamma (g_{0F} - g_{1F}) & 1 + A_F g_{0F} + 12 \Delta\gamma g_{1F} \end{pmatrix}$$

$$\hat{t}_{2F} = \hat{t}_{3F} = \hat{t}_{4F} = \frac{1}{F_{PF}} \quad , \hat{t}_{5F} = \hat{t}_{6F} = \frac{1}{F_{DF1}} \quad ,$$

$$\hat{t}_{7F} = \hat{t}_{8F} = \hat{t}_{9F} = \frac{1}{F_{DF2}} \quad , \text{ and } \hat{t}_{10F} = \hat{t}_{11F} = \hat{t}_{12F} = \frac{1}{F_{FF}} \quad ; \qquad (4.19)$$

where,

$$A_F = \Delta M \omega^2 - 12 \Delta \gamma \quad , \qquad (4.20)$$

$$m_F = A_F g_{1F} + \Delta\gamma (g_{0F} + g_{5F} + 2g_{2F} + 4g_{1F} + 4g_{4F}) \ , \qquad (4.21)$$

$$F_{SF} = (1 + \Delta M \omega^2 g_{1F} - m_F)(1 + A_F g_{0F} + 12 \Delta\gamma g_{1F}) - 12 \Delta\gamma m_F (g_{0F} - g_{1F}) \quad , \qquad (4.22)$$

$$F_{PF} = 1 + \Delta\gamma (- g_{0F} - 2g_{1F} + 2g_{4F} + g_{5F}) \quad , \qquad (4.23)$$

$$F_{DF1} = 1 + \Delta\gamma (- g_{0F} + 2g_{1F} - 2g_{2F} + 2g_{4F} - g_{5F}) \quad , \qquad (4.24)$$

$$F_{DF2} = 1 + \Delta\gamma (- g_{0F} + 2g_{2F} - g_{5F}) \quad , \qquad (4.25)$$

and ,

$$F_{FF} = 1 + \Delta\gamma (- g_{0F} + 2g_{1F} - 2g_{4F} + g_{5F}) \quad . \qquad (4.26)$$

The scattering amplitude in this case can be written in the form,

$$f_F(\underline{k}, \underline{k}_o) = f_{SF}(\underline{k}, \underline{k}_o) + f_{PF}(\underline{k}, \underline{k}_o) + f_{DF1}(\underline{k}, \underline{k}_o) + f_{DF2}(\underline{k}, \underline{k}_o) + f_{FF}(\underline{k}, \underline{k}_o) \quad , \qquad (4.27)$$

where,

$$f_{SF}(\underline{k},\underline{k}_o) = \frac{g_F(\underline{k}_o)}{F_{SF}} \Big[(1 + \Delta M \,\omega^2 g_{1F} - m_F) \Big\{ A_F + 4\Delta\gamma'(C_1C_2 + C_2C_3 + C_3C_1) \Big\} - 4\Delta\gamma' m_F(3 - C_1C_2 - C_2C_3 - C_3C_1)$$

$$+ 4\Delta\gamma' (C_{o1} C_{o2} + C_{o2}C_{o3} + C_{o3}C_{o1}) \times$$

$$\Big\{ \frac{1}{3} (1 + A_F g_{OF} + 12\Delta\gamma' g_{1F}) (3 - C_1C_2 - C_2C_3 - C_3C_1)$$

$$- (g_{OF} - g_{1F}) \big[A_F + 4\Delta\gamma'(C_1C_2 + C_2C_3 + C_3C_1) \big] \Big\} \Big] \qquad (4.28\ )$$

$$f_{PF}(\underline{k} ,\underline{k}_o) = - \frac{2\Delta\gamma'}{F_{PF}} g_F(\underline{k}_o) \Big[S_1(C_2 + C_3)S_{o1}(C_{o2} + C_{o3})$$

$$+ S_2(C_3 + C_1)S_{o2}(C_{o3} + C_{o1})$$

$$+ S_3 (C_1 + C_2)S_{03}(C_{o1} + C_{o2}) \Big] \qquad (4.29\ )$$

$$f_{DF1}(\underline{k},\underline{k}_o) = \frac{2}{3} \frac{\Delta\gamma'}{F_{DF1}} g_F(\underline{k}_o) \Big[3(C_3C_1 - C_1C_2)(C_{o3}C_{o1} - C_{o1}C_{o2})$$

$$+(2C_2C_3 - C_3C_1 - C_1C_2)(2C_{o2}C_{o3} - C_{o3}C_{o1} - C_{o1}C_{o2}) \Big] \qquad (4.30)$$

$$f_{DF2}(\underline{k} ,\underline{k}_o) = \frac{4\Delta\gamma'}{F_{DF2}} g_F(\underline{k}_o) \Big[S_1S_2S_{o1}S_{o2} + S_2S_3S_{o2}S_{o3}$$

$$+ S_3S_1S_{o3}S_{o1} \Big] \ . \qquad (\ 4.31\ )$$

and,

$$f_{FF}(\underline{k} ,\underline{k}_o) = - \frac{2\Delta\gamma'}{F_{FF}} g_F (\underline{k}_o) \Big[S_1 (C_2 - C_3)S_{01}(C_{o2} - C_{o3})$$

$$+ S_2(C_3 - C_1)S_{o2}(C_{o3} - C_{o1})$$

$$+ S_3(C_1 - C_2)S_{o3}(C_{o1} - C_{o2}) \Big] \ . \qquad (4.32)$$

Here we have distinguished between the two D-wave amplitudes f_{DF1} and f_{DF2} that arise due to the two irreducible representations E_g and F_{2g} of O_h. This identification is described in the character table given in Appendix III. It may be noted that f_{DF1} above is very similar to f_D for the simple cubic lattice given by equation (3.15). This may be expected due to the fact that both of them arise due to the irreducible representation E_g of O_h . At the same time, f_{DB} is very similar to f_{DF2}, both arising from the irreducible representation F_{2g}.

For the isotopic impurity case only the S-wave amplitude remains in both cases, and the form of the amplitude is the same as that in the simple cubic lattice given by equations (3.16) and (3.17) .

§ 4.3 The scattering cross-section, its long wavelength limit and resonances

As mentioned in the last chapter, $\underline{k}$ specifies the incident direction and $\underline{k}_o$, the direction of scattering whenever $\underline{k}_o$ is along any of the symmetry axes. The total scattering cross-section is found by using the Optical Theorem. An interesting feature of the scattering process is that the number of partial waves that contribute to the total scattering cross-section depends on the direction of incidence of the phonon. This is expected, in view of the fact that the 'potential' due to the impurity is a non-central one, and its 'range' depends on the direction in which it is viewed. We will discuss the results for the total scattering cross-sections corresponding to a few incident directions to demonstrate this effect.

The forward scattering amplitude, which is necessary for the use of the Optical Theorem to evaluate the total scattering cross section, is easily found when the direction of incidence is (100), (110) or (111). One can then set $\underline{k} = \underline{k}_0$. For incidence along (100) direction,

$$\underline{k} = \underline{k}_0 = (k,0,0,)$$

and in the Body Centred Cubic lattice,

$$g_B(\underline{k}_0) = \frac{1}{8\pi\gamma} \sec(k/2),$$

and

$$\sigma^{(100)}_{TB} = \frac{1}{4\gamma \operatorname{Sin}\frac{k}{2}} \left[\frac{1}{|F_{SB}|^2} \left\{ (\operatorname{Im} D_{B1})(\operatorname{Re} F_{SB}) - (\operatorname{Re} D_{B1})(\operatorname{Im} F_{SB}) \right\} + \frac{8(\Delta\gamma)}{|F_{PB}|^2} \sin^2(k/2).(\operatorname{Im} F_{PB}) \right] \tag{4.33}$$

in units of a^2. Here D_{B1} is given by,

$$D_{B1} = (1 + \Delta M\omega^2 g_{1B} - m_B)(A_B + 8\Delta\gamma\cos k/2) - 8\Delta\gamma m_B(1 - \cos k/2) + 8\Delta\gamma\cos(k/2)\left\{(1 - \cos k/2)(1 + A_B g_{0B} + 8\Delta\gamma g_{1B}) - (g_{0B} - g_{1B})(A_B + 8\Delta\gamma\cos k/2)\right\} . \tag{4.34}$$

$\sigma^{(100)}_{TB}$ shows no D and F wave contributions. For (111) direction,

$$\underline{k} = \underline{k}_0 = (k/3^{\frac{1}{2}},\ k/3^{\frac{1}{2}},\ k/3^{\frac{1}{2}}),$$

and,

$$\sigma^{(111)}_{TB} = \frac{1}{2\gamma(12)^{\frac{1}{2}} \operatorname{Sin}(k/12^{\frac{1}{2}}) \operatorname{Cos}^2(k/12^{\frac{1}{2}})} \left[\frac{1}{|F_{SB}|^2} \left\{ (\operatorname{Im} D_{B2})(\operatorname{Re} F_{SB}) - (\operatorname{Re} D_{B2})(\operatorname{Im} F_{SB}) \right\} + \frac{24\Delta\gamma}{|F_{PB}|^2} \cos^4(k/12^{\frac{1}{2}}) \sin^2(k/12^{\frac{1}{2}}) (\operatorname{Im} F_{PB}) - \frac{24\Delta\gamma}{|F_{DB}|^2} \cos^2(k/12^{\frac{1}{2}}) \sin^4(k/12^{\frac{1}{2}}) (\operatorname{Im} F_{DB}) + \frac{8\Delta\gamma}{|F_{FB}|^2} \sin^6(k/12^{\frac{1}{2}}) (\operatorname{Im} F_{FB}) \right] , \tag{4.35}$$

in units of a^2. Here D_{B2} is given by,

$$\begin{aligned} D_{B2} = {} & (1 + \Delta M\,\omega^2 g_{1B} - m_B)(\Lambda_B + 8\Delta\gamma \cos^3 k/12^{\frac{1}{2}}) \\ & - 8\Delta\gamma m_B(1 - \cos^3 k/12^{\frac{1}{2}}) + 8\Delta\gamma \cos^3 k/12^{\frac{1}{2}} \times \\ & \Big\{(1 - \cos^3 k/12^{\frac{1}{2}})(1 + \Lambda_B g_{0B} + 8\Delta\gamma g_{1B}) \\ & - (g_{0B} - g_{1B})(\Lambda_B + 8\Delta\gamma \cos^3 k/12^{\frac{1}{2}})\Big\} . \qquad (4.36) \end{aligned}$$

Thus $\sigma^{(111)}_{TB}$ shows contributions from all the partial waves.

For (110) direction, it can be shown that the F wave contribution is suppressed.

In the face centred cubic lattice the corresponding expressions for the total scattering cross section can be found in the same way. For example,

$$\begin{aligned} \sigma^{(110)}_{TF} = {} & \frac{1}{2\gamma\,(8)^{\frac{1}{2}}(\sin k/8^{\frac{1}{2}})(1 + \cos k/8^{\frac{1}{2}})}\Bigg[\frac{1}{|F_{SF}|^2} \times \\ & \Big\{(\mathrm{Im}\, D_F)(\mathrm{Re}\, F_{SF}) - (\mathrm{Re}\, D_F)(\mathrm{Im}\, F_{SF})\Big\} \\ & + \frac{4\Delta\gamma}{|F_{PF}|^2} \sin^2 k/8^{\frac{1}{2}}(1 + \cos k/8^{\frac{1}{2}})^2(\mathrm{Im}\, F_{PF}) \\ & - \frac{8\Delta\gamma}{|F_{DF1}|^2} \cos^2 k/8^{\frac{1}{2}}(1 - \cos k/8^{\frac{1}{2}})^2(\mathrm{Im}\, F_{DF1}) \\ & - \frac{4\Delta\gamma}{|F_{DF2}|^2} \sin^4 k/8^{\frac{1}{2}}(\mathrm{Im}\, F_{DF2}) \\ & + \frac{4\Delta\gamma}{|F_{FF}|^2} \sin^2 k/8^{\frac{1}{2}}(1 - \cos k/8^{\frac{1}{2}})^2(\mathrm{Im}\, F_{FF})\Bigg] \qquad (4.37) \end{aligned}$$

in units of a^2, with D_F given by,

$$\begin{aligned} D_F = {} & (1 + \Delta M\,\omega^2 g_{1F} - m_F)\Big\{\Lambda_F + 4\Delta\gamma(2\cos k/8^{\frac{1}{2}} + \cos^2 k/8^{\frac{1}{2}})\Big\} \\ & - 4\Delta\gamma m_F(3 - 2\cos k/8^{\frac{1}{2}} - \cos^2 k/8^{\frac{1}{2}}) + 4\Delta\gamma(2\cos k/8^{\frac{1}{2}} + \cos^2 k/8^{\frac{1}{2}}) \times \end{aligned}$$

$$\Big\{ \frac{1}{3} (1 + A_F g_{0F} + 12 {}_{\wedge}^{\Delta\gamma} g_{1F})(3 - 2 \cos k/8^{\frac{1}{2}} - \cos^2 k/8^{\frac{1}{2}}) - (g_{0F} - g_{1F}) \left[A_F + 4\Delta\gamma (2 \cos k/8^{\frac{1}{2}} + \cos^2 k/8^{\frac{1}{2}}) \right] \Big\} \quad (4.38)$$

Similar expressions can be obtained for incidence along (100) and (111) directions. Table I gives the number of partial waves contributing to the total scattering cross section for various directions of incidence in simple cubic, body centred cubic and face centred cubic lattices.

Table I

Crystallographic axes of incidence	Partial Waves Contributing to σ_T		
	Simple cubic	B.C.C.	F.C.C.
(100)	S, P and D	S and P	S, P and D_1
(110)	S, P and D	S, P and D	S, P, D_1, D_2, F
(111)	S and P	S, P, D, F	S, P and D_2

In the limit of long waves the dependence of the total scattering cross section on the incident direction ceases to exist, as expected, and the expressions for the two lattices are (in units of a^2),

$$\sigma_{TB} = \frac{4}{\pi |F_{SB}|^2} \left(\frac{\omega}{\omega_{0B}}\right)^4 \left(\frac{\Delta M}{M}\right)^2 \left[1 + \left(\frac{\Delta\gamma}{\gamma}\right)\right]^2 + \frac{16}{3\pi |F_{PB}|^2} \left(\frac{\omega}{\omega_{0B}}\right)^4 \left(\frac{\Delta\gamma}{\gamma}\right)^2 . \quad (4.39)$$

$$\sigma_{TF} = \frac{1}{4\pi |F_{SF}|^2} \left(\frac{\omega}{\omega_{0F}}\right)^4 \left(\frac{\Delta M}{M}\right)^2 \left[1 + \left(\frac{\Delta\gamma}{\gamma}\right)\right]^2 + \frac{1}{3\pi |F_{PF}|^2} \left(\frac{\omega}{\omega_{0F}}\right)^4 \left(\frac{\Delta\gamma}{\gamma}\right)^2 \quad (4.40)$$

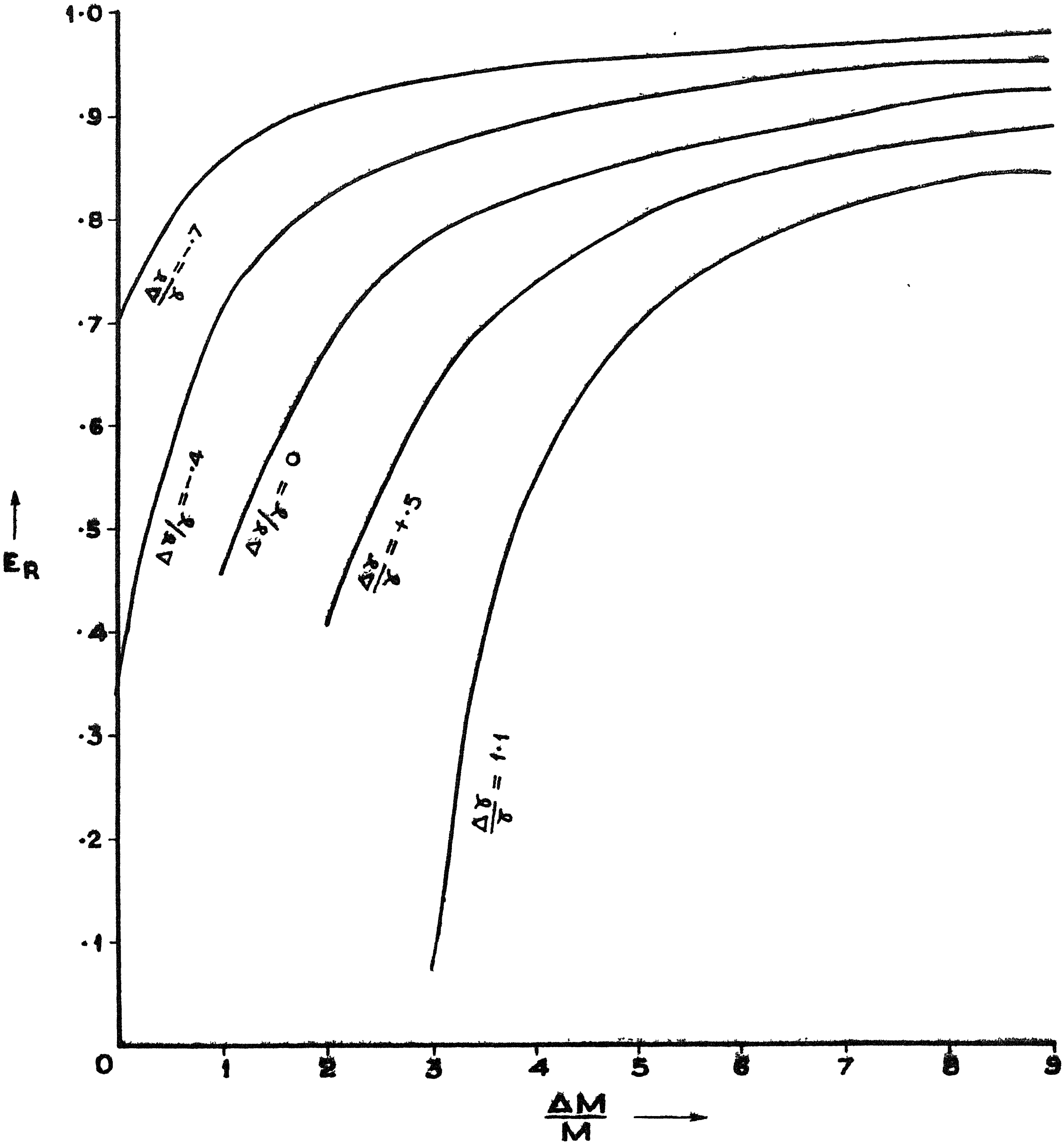


FIGURE 7 TYPICAL S-WAVE RESONANCES IN B.C.C.

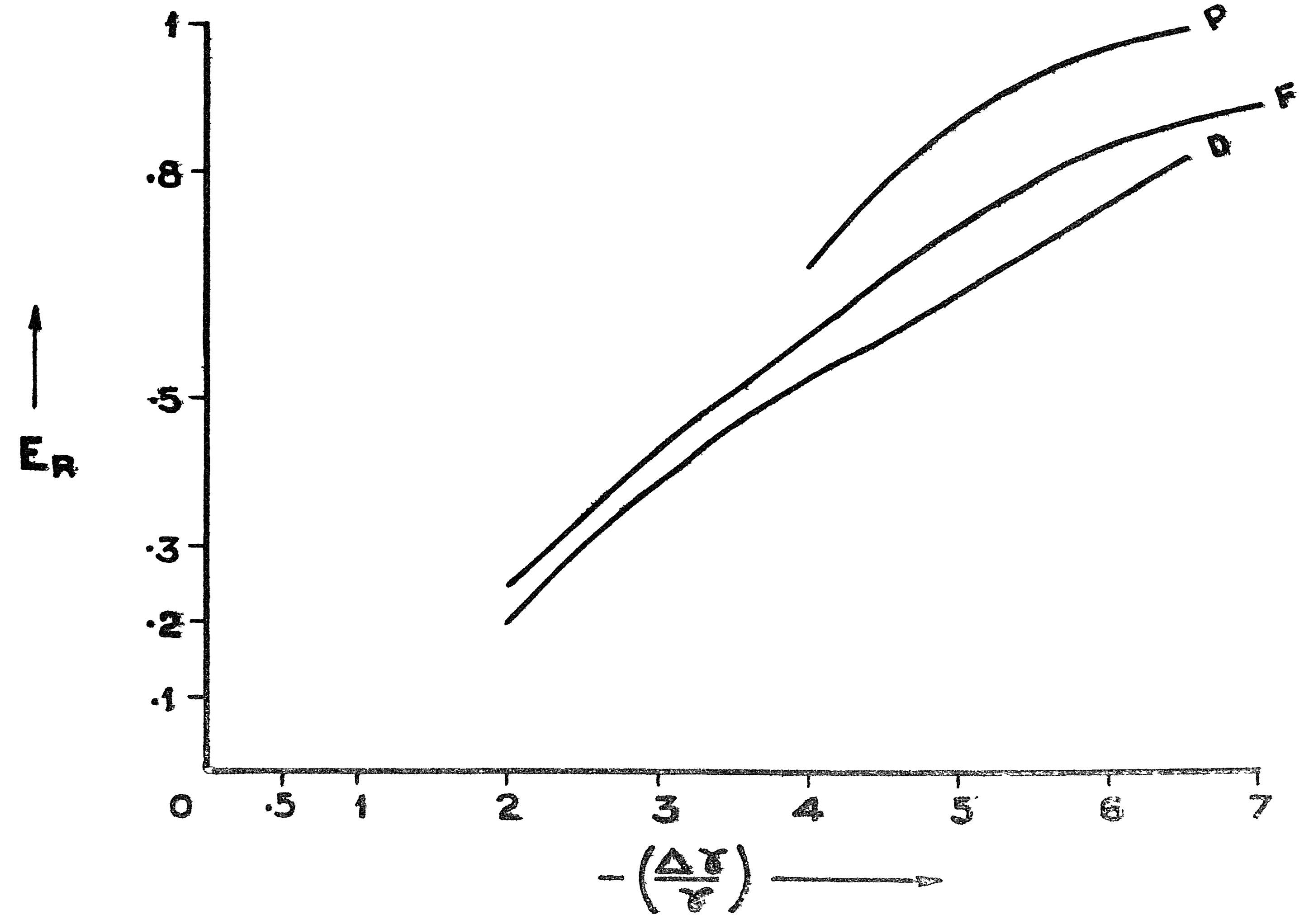


FIGURE: 8. **TYPICAL P,D,F. WAVE RESONANCES IN B.C.C.**

The scattering cross section in both cases reveals Rayleigh-type scattering when there is no resonance. F_{SF} and F_{PF} are to be evaluated in the low frequency limit. The change of mass affects only the S wave part, and the change in force constants affects all the partial waves.

As discussed in the last chapter, this Rayleigh-type of scattering does not hold at resonances. At a certain frequency ω_r, the total cross section will be proportional to ω_r^4 in absence of resonance but at resonance it will be much larger and will be proportional to ω_r^{-2}. This is because when there is a S-type of resonance, the Re $Fs_{B,F}$ will vanish and Im $Fs_{B,F}$ is proportional to $\left(\frac{\omega}{\omega_{OB,F}}\right)^3$ so that $\sigma_{TB,F}$ is proportional to $\left(\frac{\omega}{\omega_{OB,F}}\right)^{-2}$. Thus the total cross section becomes larger by a factor $\left(\frac{\omega}{\omega_{OB,F}}\right)^{-6}$. The same is true for the P- wave resonances where Re $F_{PB,F} = 0$ and Im $F_{PB,F}$ is proportional to $\left(\frac{\omega}{\omega_{OB,F}}\right)^3$. The width of these resonances will be Γ_ω given by equation (2.43). It is seen easily that Γ_ω is proportional to $\left(\frac{\omega}{\omega_{OB,F}}\right)^3$.

The resonances in the scattering cross section can be investigated in the same way as in chapter III. The figures 7 & 8 show the results for body centred cubic lattice. Here E_R denotes the value of E_B (defined in Appendix I) at resonance.

From the figures one can see that the P , D and F- like resonances occur only when the force constants are decreased sufficiently. These of course do not involve the change in mass. The S-wave resonances depend on ΔM and $\Delta\gamma$. For slight increase in mass and sufficient decrease in the force constant one obtains resonances. For very high value of the increase in mass, resonances appear near the band edge, no matter whether the force constant is increased of decreased whereas for slight changes in mass the change in force constant plays a dominant role. The localized modes can be investigated using these resonance denominators outside the band .

§ 4.4 Phonon Scattering and the mean free path

The mean free path of phonons can be computed using equation (2.48) . This involves $\sigma_D(\theta)$ and the scattering angle θ . $\sigma_D(\theta)$ is readily computed from the scattering amplitudes. In the long wavelength limit only the S and P terms are significant upto the order ω^4 . The expressions for the scattering amplitudes for the two lattices in this limit are as follows.

(a) Body Centred Cubic lattice:

$$f(\theta) = \left[\frac{1}{\pi}\left(\frac{\Delta M}{M}\right)\left(\frac{1}{F_{SB}}\right)\left(1 + \frac{\Delta\gamma}{\gamma}\right) - \frac{2}{\pi}\left(\frac{1}{F_{PB}}\right) \times \frac{\Delta\gamma}{\gamma} \cos\theta \right] \left(\frac{\omega}{\omega_{OB}}\right)^2 \tag{4.41}$$

which, when substituted in equation (2.48) , gives us,

$$\frac{1}{\Lambda(\omega)} = 16\, N_c\, a^2 \left(\frac{\omega}{\omega_{OB}}\right)^4 \left[\frac{1}{4\pi|F_{SB}|^2}\left(\frac{\Delta M}{M}\right)^2\left(1 + \frac{\Delta\gamma}{\gamma}\right)^2 + \frac{1}{3\pi|F_{PB}|^2}\left(\frac{\Delta\gamma}{\gamma}\right)^2 + \frac{1}{6\pi}\left(\frac{\Delta\gamma}{\gamma}\right)\left(\frac{\Delta M}{M}\right)\left(1 + \frac{\Delta\gamma}{\gamma}\right) \times \left\{ \frac{1}{F^*_{SB}\,F_{PB}} + \frac{1}{F_{SB}\,F^*_{PB}} \right\} \right]. \tag{4.42}$$

(b) Face Centred Cubic lattice:

$$f(\theta) = \left\{ \frac{1}{4\pi} \left[\frac{\Delta M}{M} \right] \left[\frac{1}{F_{SF}} \right] \left[1 + \frac{\Delta \gamma}{\gamma} \right] - \frac{1}{2\pi} \left(\frac{\Delta \gamma}{\gamma} \right) \left(\frac{1}{F_{PF}} \right) \cos \theta \right\} \left(\frac{\omega}{\omega_{OF}} \right)^2 , \qquad (4.43)$$

and proceeding in the same way we obtain,

$$\frac{1}{\Lambda(\omega)} = N_c a^2 \left(\frac{\omega}{\omega_{OF}} \right)^4 \left[\frac{1}{4\pi |F_{SF}|^2} \left(\frac{\Delta M}{M} \right)^2 \left(1 + \frac{\Delta \gamma}{\gamma} \right)^2 + \frac{1}{3\pi |F_{PF}|^2} \left(\frac{\Delta \gamma}{\gamma} \right)^2 + \frac{1}{6\pi} \left(\frac{\Delta \gamma'}{\gamma} \right) \left(\frac{\Delta M}{M} \right) \left(1 + \frac{\Delta \gamma'}{\gamma'} \right) \left\{ \frac{1}{F_{SF}^{*} F_{PF}} + \frac{1}{F_{SF} F_{PF}^{*}} \right\} \right] \qquad (4.44)$$

It may be noted that in the expression for the mean free path the two partial waves lead to an interference term like the one given by equation (3.34) for the simple cubic lattice.

In conclusion, it may be stated that even in the somewhat unrealistic models of cubic lattices studied here, some important features of the scattering process of phonons from a substitutional impurity become evident. The total scattering cross section depends on the direction of incidence of the phonons, as also the number of partial waves that contribute to the cross section. But in the limit of long waves, no such dependence is there due to the isotropy of the constant frequency surfaces. The dispersion laws of the models considerdd here lead to Debye model in this limit. The mean free path for long wave phonons contains terms that arise due to the interference of S and P partial waves. A comparison of the results obtained in this chapter with those obtained in the last chapter shows a great deal of similarity among the three types of cubic lattices.

CHAPTER V

A MODEL WITH PHONON POLARIZATION

§ 5.1 Introduction

The process of the scattering of phonons from a substitutional impurity considered in this chapter includes the polarization of phonons in the lattice. This problem has been discussed briefly by Thoma and Ludwig [13] for the isotope defect. Maradudin[45] has treated the isotope defect case in some detail and derived the scattering cross section in the limit of long waves by using Debye approximation. Here we treat this isotope defect case in detail without using Debye approximation in the limit of long waves and then we discuss the problem for a general substitutional impurity with group theoretical partial wave analysis which has been done for the scalar models in the last two chapters.

The problem is mathematically involved in the sense that significant part of the calculation requires cumbersome numerical work. Physically the process is complex because here the concept of polarization of phonons is not as simple as in the familiar case of photons. In general each state of polarization of phonons corresponds to a dispersion law peculiar to that state, unlike the case of photons where all the polarization states correspond to the same dispersion. All these dispersions become identical if for example the model is such that one Cartesian component of the displacement of any atom is not influenced by the other Cartesian components of displacements of the same atom or its neighbours. In chapter III we considered such a model.

The scattering problem can be stated as follows. Let phonons with a definite polarization and hence corresponding to a definite frequency branch be incident on a defect site and get scattered. In general they will get scattered into other states of polarization also. As expected the scattering process depends strongly upon the incident direction. It is required to find out the scattering cross sections for the process. In the model that will be considered here, the constant frequency surface at low frequencies will not be spherical as is the case with the usual assumption of Debye approximation in this limit.

§ 5.2 The model

A monoatomic body centred cubic lattice is considered in which each atom has mass M and is coupled to its nearest neighbours through central and non-central harmonic force constants γ_1 and γ_2 respectively. Such a model has been discussed by Fine[46] and subsequently by Launay[44]. The main assumptions and approximations involved are the same as discussed in chapter II and the Cartesian Co-ordinate system is identical to that described in the last chapter for the body centred cubic lattice. A general substitutional impurity is put at the origin whose mass is $M + \Delta M$ and which is coupled to its nearest neighbours through force constants $\gamma_1 + \Delta\gamma_1$ and $\gamma_2 + \Delta\gamma_2$. The total number of atoms is taken to be N. γ_1 and γ_2 are supposed to be unequal because if they are equal one gets results identical to those obtained in the last chapter. This is due to the fact that when $\gamma_1 = \gamma_2$, then for example the Cartesian X - component of the displacement of an atom is not coupled to the Y or Z components of the displacements of the same atom or its nearest neighbours. Thus to make a transition to the scalar model from this, one has to set $\gamma_1 = \gamma_2$.

The time independent equations of motion can be written in the matrix form [47] (we shall write $\underline{U}(\underline{k};\underline{R})$ as $U(\underline{R})$ in this chapter)

$$\hat{D}\underline{U} - M\omega^2\underline{U} = 0 \qquad (5.1)$$

where $\hat{D}$ is $3N \times 3N$ matrix and $\underline{U}$ is $3N$ - dimensional vector. We shall follow the following partitioning. $\underline{U}$ is partitioned into three N - dimensional vectors $\underline{U}_\alpha$, $\alpha = 1,2,3$ such that $\underline{U}_1$ has the X-displacements of all the N atoms as its elements. Also $\hat{D}$ is partitioned into the corresponding $N \times N$ blocks $\hat{D}_{\alpha\beta}$ each of which is a cyclic matrix. Using ℓ , m, n defined through equation (4.1a), i.e.,

$$\underline{R} = \left(\ell + \frac{m}{2}\right) a\,\underline{e}_1 + \frac{m}{2}\, a\,\underline{e}_2 + \left(\frac{m}{2} + n\right) a\,\underline{e}_3$$

and defining the two constants

$$\beta_1 = \left(\frac{\gamma_1 + 2\gamma_2}{3}\right) \quad \text{and} \quad \beta_2 = \left(\frac{\gamma_1 - \gamma_2}{3}\right)$$

the elements of $\hat{D}_{\alpha\beta}$ can be written as follows,

$$\begin{aligned} D_{\alpha\alpha}&(\ell mn, \ell'm'n') \\ = \beta_1\Big[& 8\,\delta_{\ell',\ell}\,\delta_{m',m}\,\delta_{n',n} - \delta_{\ell',\ell}\,\delta_{n',n}\big\{\delta_{m',m+1} \\ & + \delta_{m',m-1}\big\} - \delta_{n,n'}\big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1} \\ & + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\big\} - \delta_{\ell',\ell}\big\{\delta_{m',m+1}\,\delta_{n',n-1} \\ & + \delta_{m',m-1}\,\delta_{n',n+1}\big\} - \big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1}\,\delta_{n',n+1} \\ & + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\,\delta_{n',n-1}\big\}\Big] \end{aligned} \qquad (5.2)$$

for $\alpha = 1,2$ and 3.

Also

$$D_{12}(\ell mn, \ell'm'n') = D_{21}(\ell mn, \ell'm'n')$$

$$\begin{aligned} &= \beta_2 \Big[\delta_{\ell',\ell}\,\delta_{n',n}\left(\delta_{m',m+1} + \delta_{n',m-1}\right) + \delta_{\ell',\ell}\Big\{\delta_{m',m+1}\,\delta_{n',n-1} \\ &\quad + \delta_{m',m-1}\,\delta_{n',n+1}\Big\} - \delta_{n'n}\Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\Big\} - \Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1}\,\delta_{n',n+1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\,\delta_{n',n-1}\Big\}\Big] \end{aligned} \tag{5.3}$$

$$D_{13}(\ell mn, \ell'm'n') = D_{31}(\ell mn, \ell'm'n')$$

$$\begin{aligned} &= \beta_2 \Big[\delta_{\ell',\ell}\,\delta_{n',n}\left(\delta_{m',m+1} + \delta_{m',m-1}\right) - \delta_{\ell',\ell}\Big\{\delta_{m',m+1}\,\delta_{n',n-1} \\ &\quad + \delta_{m',m-1}\,\delta_{n',n+1}\Big\} + \Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1}\,\delta_{n',n+1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\,\delta_{n',n-1}\Big\} - \delta_{n',n}\Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\Big\}\Big] \end{aligned} \tag{5.4}$$

and

$$D_{23}(\ell mn, \ell'm'n') = D_{32}(\ell mn, \ell'm'n')$$

$$\begin{aligned} &= \beta_2 \Big[\delta_{\ell',\ell}\,\delta_{n',n}\Big\{\delta_{m',m+1} + \delta_{m',m-1}\Big\} - \delta_{\ell',\ell}\Big\{\delta_{m',m+1}\,\delta_{n',n-1} \\ &\quad + \delta_{m',m-1}\,\delta_{m',n+1}\Big\} - \Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1}\,\delta_{n',n+1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\,\delta_{n',n-1}\Big\} + \delta_{n',n}\Big\{\delta_{\ell',\ell+1}\,\delta_{m',m-1} \\ &\quad + \delta_{\ell',\ell-1}\,\delta_{m',m+1}\Big\}\Big] \end{aligned} \tag{5.5}$$

The solution of equation (5.1) is denoted by $\underline{U}_o$.

Substituting.

$$U_\alpha(R) = v_\alpha \exp(i\,\underline{k}\cdot\underline{R})$$

in equation (5.1) leads to the equations

$$\sum_{\beta} \sigma^{(k)}_{\alpha\beta} v_{\beta} - M \omega^{2} v_{\alpha} = 0 \qquad (5.6)$$

where $$\sigma^{(k)}_{\alpha\beta} = \sum_{\underline{R}'} D_{\alpha\beta}(\underline{R}, \underline{R}') \exp\{i\, \underline{k}.(\underline{R}' - \underline{R})\}$$

defines the elements of the dynamical matrix σ . Thus equation (5.6) becomes ,

$$\sigma v = M \omega^{2} v \qquad (5.7)$$

which is an eigenvalue equation. This gives three eigenvalues $M\omega^{2}_{j}(\underline{k})$, $j = 1,2,3$ which are the three frequency branches and the corresponding eigenvectors v denoted by $e^{(j)}(\underline{k})$ with components $e^{(j)}_{\alpha}(\underline{k})$, $j, \alpha = 1,2$ and 3 ; are the polarization vectors for phonon propagating with wave vector $\underline{k}$. For the model under consideration, the σ matrix has the explicit form,

$$\sigma = \begin{bmatrix} 8\beta_1(1-C_1C_2C_3) & 8\beta_2 S_1S_2C_3 & 8\beta_2 S_1C_2S_3 \\ 8\beta_2 S_1S_2C_3 & 8\beta_1(1-C_1C_2C_3) & 8\beta_2 C_1S_2S_3 \\ 8\beta_2 S_1C_2S_3 & 8\beta_2 C_1S_2S_3 & 8\beta_1(1-C_1C_2C_3) \end{bmatrix} \qquad (5.8)$$

with $S_i = \sin \frac{k_i}{2}$ and $C_i = \cos \frac{k_i}{2}$.

The eigenvalues $M\omega^{2}_{j}(\underline{k})$ are found from the roots of the cubic equation,

$$\lambda^{3} - (8\beta_2)^{2}\left\{S_1^2S_2^2C_3^2 + S_1^2C_2^2S_3^2 + C_1^2S_2^2S_3^2\right\}\lambda + 2(8\beta_2)^{3}\left(S_1^2S_2^2S_3^2C_1C_2C_3\right) = 0 \qquad (5.9)$$

with the roots λ_j , $j = 1,2,3$ related to the eigenvalues as

$$\lambda_j = 8\beta_1(1 - C_1C_2C_3) - M\omega^{2}_{j}(\underline{k}) \qquad (5.10)$$

Then the eigenvectors $\underline{e}^{(j)}(\underline{k})$ are ,

$$e^{(j)}(\underline{k}) = \begin{bmatrix} \left\{8\beta_2\left(S_1S_2C_3 + S_1C_2S_3 - C_1S_2S_3\right) - \lambda_j\right\}\left\{\lambda_j - 8\beta_2\, C_1S_2S_3\right\}/D_j \\ \left\{8\beta_2\left(C_1S_2S_3 + S_1S_2C_3 - S_1C_2S_3\right) - \lambda_j\right\}\left\{\lambda_j - 8\beta_2\, S_1C_2S_3\right\}/D_j \\ \left\{8\beta_2\left(S_1C_2S_3 + C_1S_2S_3 - S_1S_2C_3\right) - \lambda_j\right\}\left\{\lambda_j - 8\beta_2\, S_1S_2C_3\right\}/D_j \end{bmatrix} \tag{5.11}$$

with j = 1,2,3 and D_j are proper normalization factors.

The polarization vectors satisfy the orthonormality and closure relations ,

$$\sum_{\alpha} e_{\alpha}^{*(j)}(\underline{k})\; e_{\alpha}^{(j')}(\underline{k}) = \delta_{jj'} \tag{5.12}$$

and
$$\sum_{j} e_{\alpha}^{*(j)}(\underline{k})\; e_{\beta}^{(j)}(\underline{k}) = \delta_{\alpha\beta} \tag{5.13}$$

and products like $e_{\alpha}^{(j)}(\underline{k})\; e_{\beta}^{*(j)}(\underline{k})$ transform as $k_\alpha k_\beta$ under the symmetry operations of the point group of the crystal under which $\omega_j^2(\underline{k})$ remain invariant.

Now let the substitutional impurity be put at the origin of the co-ordinate system. The equation of motion will now read as,

$$\hat{D}\,\underline{U} - M\omega^2\,\underline{U} = \hat{P}\,\underline{U} \tag{5.14}$$

whose general solution will be

$$\underline{U} = \underline{U}_0 - \hat{G}\hat{P}\underline{U} \tag{5.15}$$

where the Green function $\hat{G}$ has elements given by[47]

$$G_{\alpha\beta}(\omega^2, \underline{R}, \underline{R}') = \frac{1}{NM}\sum_{\underline{k}}\sum_{j}\frac{e_{\alpha}^{*(j)}(\underline{k})\; e_{\beta}^{(j)}(\underline{k})\; \exp\left\{i\underline{k}\cdot(\underline{R}' - \underline{R})\right\}}{\omega^2 - \omega_j^2(\underline{k}) + i\epsilon} \tag{5.16}$$

In particular, $G_{\alpha\beta}(\omega^2, \underline{0}, \underline{0})$ is diagonal in α, β for the present model due to the transformation properties of $e_{\alpha}^{(j)}(\underline{k})\; e_{\beta}^{*(j)}(\underline{k})$ under the symmetry operations of O_h, the point group of the crystal under consideration.

Thus [47]

$$G_{\alpha\beta}(\omega^2,\underline{0},\underline{0}) = \frac{1}{3NM}\,\delta_{\alpha\beta}\sum_{\underline{k}}\sum_{j}\frac{1}{\omega^2-\omega_j^2(\underline{k})+i\epsilon} \qquad (5.17)$$

$$\equiv G(\omega^2,\underline{0},\underline{0})\,,$$

which shows the equality of the three diagonal elements as well.

§ 5.3 The Isotope Defect:

From equation (5.14) one gets

$$U_\alpha(\underline{R}) = U_{o\alpha}(\underline{R}) - \sum_{\beta,\beta',\underline{R}',\underline{R}''} G_{\alpha\beta}(\omega^2,\underline{R},\underline{R}')\,P_{\beta\beta'}(\underline{R}',\underline{R}'')\,U_{\beta'}(\underline{R}'') \qquad (5.18)$$

Now let the substitutional impurity be an isotope of the normal atom. Then $\Delta\gamma_1 = \Delta\gamma_2 = 0$, and the perturbation matrix $\hat{P}$ has non - vanishing elements corresponding to the defect site which is taken to be the origin. Noting that $\hat{G}$ and $\hat{P}$ have been partitioned in the same way as $\hat{D}$ one has,

$$P_{\beta\beta'}(\underline{R}',\underline{R}'') = \Delta M\omega^2\,\delta_{\beta\beta'}\,\delta_{\underline{R}',\underline{0}}\,\delta_{\underline{R}'',\underline{0}} \qquad (5.19)$$

Substituting this in equation (5.18) one gets

$$U_\alpha(\underline{R}) = U_{o\alpha}(\underline{R}) - \Delta M\omega^2\sum_{\beta} G_{\alpha\beta}(\omega^2,\underline{R},\underline{0})\,U_\beta(\underline{0}) \qquad (5.20)$$

Putting $\underline{R} = 0$ in this, one gets,

$$U_\alpha(\underline{0}) = \frac{1}{1+\Delta M\omega^2 G(\omega^2,\underline{0},\underline{0})}\,U_{o\alpha}(\underline{0}) \qquad (5.21)$$

where the fact that $G_{\alpha\beta}(\omega^2,\underline{0},\underline{0})$ is diagonal in α and β has been used. Substituting equation (5.21) back in equation (5.20) yields the result,

$$U_\alpha(\underline{R}) = U_{o\alpha}(\underline{R}) - \left[\frac{\Delta M\omega^2}{1+\Delta M\omega^2 G(\omega^2,\underline{0},\underline{0})}\right]\sum_{\beta} G_{\alpha\beta}(\omega^2,\underline{R},\underline{0})\,U_{o\beta}(\underline{0}) \qquad (5.22)$$

As discussed in Appendix II , $G_{\alpha\beta}(\omega^2, \underline{R}, \underline{0})$ can be expanded for large $\underline{R}$ as

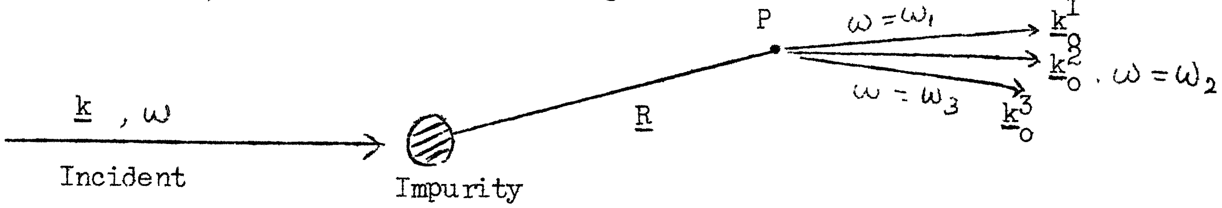
$$G_{\alpha\beta}(\omega^2, \underline{R}, \underline{0}) = -\sum_j e_\alpha^{(j)}(\underline{k}_o^j)\, g_\beta(\underline{k}_o^j)\, \frac{\exp(i\,\underline{k}_o^j\cdot\underline{R})}{R} \qquad (5.23)$$

where each term corresponds to a frequency branch denoted by the index j . Substituting this equation in equation (5.22) one gets,

$$U_\alpha(\underline{R}) = U_{o\alpha}(\underline{R}) + \sum_j e_\alpha^{(j)}(\underline{k}_o^j)\; f_i^j(\underline{k},\underline{k}_o^j)\, \frac{\exp(i\underline{k}_o^j\cdot\underline{R})}{N^{\frac{1}{2}}R} \qquad (5.24)$$

where $$f_i^j = \frac{\Delta M\omega^2}{1+\Delta M\omega^2 G(\omega^2, \underline{0},\underline{0})} \sum_\beta g_\beta(\underline{k}_o^j)\; N^{\frac{1}{2}} U_{o\beta}(\underline{0}) \qquad (5.25)$$

Here the index i refers to the polarization of the incident phonon. Thus we have the solution for the scattering problem in (5.24) for the isotope case. One can fix the incident wave by choosing $\underline{U}_o$ suitably. It is clear that for a given incident phonon with a given frequency and polarization, the scattered wave consists of in general three polarizations. Thus an incident vibration propagating in a certain direction with a given frequency and polarization is scattered from the substitutional impurity and at a large distance $\underline{R}$ the resultant vibrations can be analized into three distinct waves travelling in general in three different directions with three distinct dispersions corresponding to the given frequency of the incident vibration i,e with three different group velocities.



We shall call the three final polarizations as the three polarization channels. Equation (5.24) permits one to separate the contributions to different polarization channels. Thus, if one is interested in the scattering to the first channel (with j = 1) only, then this process is described by

$$U_{\alpha}(\underline{R}) = U_{0\alpha}(\underline{R}) + e_{\alpha}^{(1)}(\underline{k}_0^1)\, f_i^1(\underline{k}, \underline{k}_0^1)\, \frac{\exp(i\underline{k}_0^1 \cdot \underline{R})}{N^{\frac{1}{2}} R} \qquad (5.26)$$

Similarly for the channel j = 2 , one gets

$$U_{\alpha}(\underline{R}) = U_{0\alpha}(\underline{R}) + e_{\alpha}^{(2)}(\underline{k}_0^2)\, \frac{\exp(i\underline{k}_0^2 \cdot \underline{R})}{N^{\frac{1}{2}} R}\, f_i^{\,2}(\underline{k}, \underline{k}_0^2) \qquad (5.27)$$

and so on. Then these scattering amplitudes can be used to find contribution to the total scattering cross section and mean free path from phonon scattering into different channels.

However one can employ the optical theorem to find the total cross section σ_T directly. This involves the imaginary part of the forward scattering amplitude which for the present case becomes,

$$f_j^j(\underline{k}, \underline{k}) = \frac{\Delta M \omega^2}{1 + \Delta M \omega^2 G(\omega^2, \underline{0}, \underline{0})} \sum_{\beta} g_{\beta}(\underline{k})\, e_{\beta}^{(j)}(\underline{k}) \qquad (5.28)$$

where $\underline{k}$ is the incident wave vector and j is the incident polarization index.

In particular, let the phonons incident along (100) direction be considered. Then $\underline{k} = (k,0,0)$. Further let them be polarized, say longitudinally with frequency given by $\omega_1(\underline{k})$. Then we have

$$e_{\beta}^{(j)}(\underline{k}) = \delta_{\beta,1}\, \delta_{j,1} \;. \qquad (5.29)$$

and

$$f_1^1(\underline{k},\underline{k}) = \left(\frac{\Delta M \omega^2}{1 + \Delta M \omega^2 G(\omega^2, \underline{0}, \underline{0})} \right) g_1(\underline{k}) \qquad (5.30)$$

In the limit of long waves one gets for this incidence,

$$\sigma_T^{(100)} = \frac{4\pi}{k} \operatorname{Im} \left[f_1^1(\underline{k}, \underline{k}) \right]$$

$$= \frac{4\pi}{k} \left[\frac{\Delta M \omega^2 \, g_1(\underline{k})}{\left| 1 + \Delta M \omega^2 G(\omega^2, \underline{0}, \underline{0}) \right|^2} \right] \left[- \Delta M \omega^2 \operatorname{Im} G(\omega^2, \underline{0}, \underline{0}) \right] \qquad (5.31)$$

But $$g_1(\underline{k}) = \frac{2\pi^2}{\beta_1 V^*} = \frac{16\pi^2}{M V^* \omega_o^2} \qquad (5.32)$$

where $$\omega_o^2 = 8 \beta_1 / M \qquad (5.33)$$

Also $$\operatorname{Im} G(\omega^2, \underline{0}, \underline{0}) = + \frac{\operatorname{Im}}{3 NM} \sum_{\underline{k}} \sum_j \frac{1}{\omega^2 - \omega_j^2(\underline{k}) + i\epsilon}$$

$$= \frac{\operatorname{Im}}{3 M V^*} \sum_j \int \frac{d^3 k}{\omega^2 - \omega_j^2(\underline{k}) + i\epsilon}$$

$$= - \frac{\pi \omega b_1}{6 M V^* \omega_o^3} \quad \text{for small } \omega \, ; \qquad (5.34)$$

where $$b_1 = \sum_j \int \frac{\sin\theta \, d\theta \, d\varphi}{\left[F_j(\theta, \varphi) \right]^{3/2}} \qquad (5.35)$$

with $$F_j(\theta, \varphi) = \frac{1}{8} - \frac{\beta_2}{2\beta_1} \sqrt{\frac{\sin^2\theta \cos^2\theta + \sin^4\theta \cos^2\varphi \sin^2\varphi}{3}}$$

$$\times \cos\left(\frac{\lambda}{3} + \frac{2\pi j}{3} \right) , \qquad (5.36)$$

where $$\cos\lambda = \frac{(27)^{\frac{1}{2}} \sin\theta \cos^2\theta \cos^2\varphi \sin^2\varphi}{(\cos^2\theta + \sin^2\theta \cos^2\varphi \sin^2\varphi)^{3/2}} \qquad (5.37)$$

We have also to use the fact that for ,

$$\underline{k} = (k,0,0) \;,\quad M\omega^2 = \beta_1 k^2 \quad \text{or} \quad \omega^2 = \frac{k^2\omega_o^2}{8}$$

so that $$\underline{k} = \frac{2\sqrt{2}\,\omega}{\omega_o}$$

Thus finally we get

$$\sigma_T^{(100)} = \frac{4}{\pi}\left(\frac{\Delta M}{M}\right)^2 \left(\frac{\omega}{\omega_o}\right)^4 \frac{c_1}{\left|1+\Delta M\,\omega^2 G(\omega^2,\underline{0},\underline{0})\right|^2} \qquad (5.38)$$

in units of a^2,

where $$c_1 = \left[\frac{4\sqrt{2}\,\pi^5}{6\,V^{*2}}\right] b_1 = \left[\frac{\sqrt{2}}{24 \times 16\,\pi}\right] b_1 \qquad (5.39)$$

The same result is obtained for all initial polarizations with (100) , (010) and (001) incidences. This result goes over to that for the scalar model given by equation (4.39) of chapter IV (one has to set $\Delta\gamma = 0$ in this equation to get the result for isotope defect case) if we set $\beta_2 = 0$ i,e $\gamma_1 = \gamma_2$ so that $b_1 = 12\pi \times 16\sqrt{2}$ from equations (5.35), (5.36) and c_1 is unity. This transition from the present model to the scalar model by adjusting the force constants suitably is interesting to note.

The expression for σ_T above shows Rayleigh type of scattering with possibilities of resonance at which $\sigma_T \propto \omega^{-2}$. The remarkable point that emerges from this is that although the dispersion used here does not go over to Debye model dispersion in the limit of long waves like the scalar model, we still get the same result except for a numerical factor. Thus our result differs from that obtained [45] by using Debye model by a numerical factor. However, the difference lies in the fact that this numerical factor depends upon the direction of incidence and the polarization. For example, for (110) direction of incidence, c_1 in equation (5.39) must be replaced by $c_2 = c_1 \left\{ (1-\beta_2/\beta_1)(1-\beta_2/\beta_1) \right\}^{-\frac{1}{2}}$ in a typical initial choice. This reflects the departure of the present model from the Debye model in the limit of longwaves.

§ 5.4 General Defect;

Now we consider a substitutional impurity with changes in mass and force constants. Let $M + \Delta M$ be the mass of the impurity atom which is coupled to its nearest neighbours through force constants $\gamma_1 + \Delta\gamma_1$ and $\gamma_2 + \Delta\gamma_2$. The perturbation matrix $\hat{P}$ can be partitioned in the same way as $\hat{G}$ and $\hat{D}$ as,

$$\hat{P} = \begin{bmatrix} \hat{P}_{11} & \hat{P}_{12} & \hat{P}_{13} \\ \hat{P}_{21} & \hat{P}_{22} & \hat{P}_{23} \\ \hat{P}_{31} & \hat{P}_{32} & \hat{P}_{33} \end{bmatrix}$$

and each of the $N \times N$ matrices $\hat{P}_{ij}$ have non-vanishing partitions $\hat{p}_{ij}$ in the Γ - space, the space of affected lattice sites. Then one has

$$\hat{p}_{11} = \hat{p}_{22} = \hat{p}_{33} \text{ and } \hat{p}_{ij} = \hat{p}_{ji}, \quad i,j = 1,2,3$$

with $p_{11}(\underline{0},\underline{0}) = \Delta M\omega^2 - 8\Delta\beta_1$, $p_{11}(\underline{0},\underline{R}_n)$

$$= p_{11}(\underline{R}_n,\underline{0}) = \Delta\beta_1, \quad p_{11}(\underline{R}_n,\underline{R}_n) = -\Delta\beta_1, \tag{5.40}$$

$$p_{ij}(\underline{0},\underline{0}) = p_{ji}(\underline{R}_n,\underline{R}_n) = 0, \quad i \neq j$$

and $p_{ij}(\underline{0}, \underline{R}_n) = p_{ij}(\underline{R}_n, \underline{0}) = \pm \Delta\beta_2$, $i \neq j$

where the sign depends on i and j and the nearest neighbour whose lattice site is given by $\underline{R}_n$.

Here $\Delta\beta_1 = \dfrac{(\Delta\gamma_1 + 2\Delta\gamma_2)}{3}$ and $\Delta\beta_2 = \dfrac{(\Delta\gamma_1 - \Delta\gamma_2)}{3}$ (5.41)

We follow the partitioning already described and define $\underline{S} = \hat{P}\,\underline{U}$, $\underline{S}_o = \hat{P}\,\underline{U}_o$ to get the scattering equation as

$$\underline{S} = \underline{S}_o - \hat{P}\,\hat{G}\,\underline{S} \qquad (5.42)$$

whence $\underline{s}_\alpha = \underline{s}_{o\alpha} - \sum_{\beta,\beta'} \hat{p}_{\alpha\beta}\,\hat{G}_{\beta\beta'}\,\underline{s}_{\beta'}$, $\alpha = 1,2,3$ (5.43)

where $\underline{s}_\alpha$ is the only non-vanishing part of $\underline{S}_\alpha$ and lies in the Γ-space.

If we define a 27 - dimensional vector,

$$\underline{s} = \begin{bmatrix} \underline{s}_1 \\ \underline{s}_2 \\ \underline{s}_3 \end{bmatrix}, \quad \hat{p} = \begin{bmatrix} \hat{p}_{11} & \hat{p}_{12} & \hat{p}_{13} \\ \hat{p}_{21} & \hat{p}_{22} & \hat{p}_{23} \\ \hat{p}_{31} & \hat{p}_{32} & \hat{p}_{33} \end{bmatrix}$$

and $$\hat{g} = \begin{bmatrix} \hat{g}_{11} & \hat{g}_{12} & \hat{g}_{13} \\ \hat{g}_{21} & \hat{g}_{22} & \hat{g}_{23} \\ \hat{g}_{31} & \hat{g}_{32} & \hat{g}_{33} \end{bmatrix}$$

then we get

$$\underline{s} = \underline{s}_o - \hat{p}\,\hat{g}\,\underline{s} \qquad (5.44)$$

whose solution is

$$\underline{s} = (\hat{I} + \hat{p}\hat{g})^{-1}\,\underline{s}_o \qquad (5.45)$$

$$= \hat{V}^{+} \hat{M} \hat{V} \underline{s}_{o} \qquad (5.46)$$

where the $\hat{V}$ - matrix found group theoretically block diagonolizes $(\hat{I} + \hat{p}\hat{g})^{-1}$ to $\hat{M}$.

We can, as in chapter II, write $\hat{M}$ as $M = \sum_{\nu} M_{\nu}$ corresponding to different symmetry blocks and get

$$\underline{s}_{\nu} = \hat{V}^{+} \hat{M}_{\nu} \hat{V} \underline{s}_{o} \qquad (5.47)$$

so that $\underline{s} = \sum_{\nu} \underline{s}_{\nu}$

From these we obtain expressions for $\underline{s}_{\alpha}$ whence $\underline{S}_{\alpha}$ are known and then

$$\underline{U} = \underline{U}_{o} - \hat{G} \underline{S} \qquad (5.48)$$

gives

$$U_{\alpha}(\underline{R}) = U_{o\alpha}(\underline{R}) - \sum_{\beta, \underline{R}_{n}}' G_{\alpha\beta}(\omega^{2}, \underline{R}, \underline{R}_{n}) S_{\beta}(\underline{R}_{n}) \qquad (5.49).$$

For large $\underline{R}$ one can expand $G_{\alpha\beta}(\omega^{2}, \underline{R}, \underline{R}_{n})$ asymptotically to get,

$$U_{\alpha}(\underline{R}) = U_{o\alpha}(\underline{R}) + \sum_{j} e_{\alpha}^{(j)}(\underline{k}_{o}^{j}) F(\underline{k}^{i}, \underline{k}_{o}^{j}) \exp \frac{(i\underline{k}_{o}^{j} \cdot \underline{R})}{|\underline{R}| \sqrt{N}} \qquad (5.50)$$

where $\underline{k}$ and i specify the wave vector and polarization of the incident phonons and $F(\underline{k}^{i}, \underline{k}_{o}^{j})$ is some trigonometric function of $\underline{k}^{i}$ and $\underline{k}_{o}^{j}$. Then one can use the optical theorem for the total scattering cross - section. In addition to the asymptotic expansion of Green function, one needs the elements $g_{\alpha\beta}(\omega^{2}, \underline{R}_{n}, \underline{R}_{n}')$ and the $\hat{V}$ - matrix for explicit evaluation of the scattering amplitudes $F(\underline{k}^{i}, \underline{k}_{o}^{j})$ and their partial wave expansion. We proceed to discuss these in the following.

To find the $\hat{V}$ - matrix we must find the representation Γ of O_h in the space of the displacements of the impurity and its nearest neighbours. For the model under consideration, this space is twentyseven dimensional. However it is the direct product of a three dimensional space consisting of the Cartesian components of a displacement and a nine dimensional space consisting of the position co-ordinates of the affected lattice sites. Hence Γ is a direct product of Γ_1, the representation of O_h in the (x , y , z) space and Γ_2 which is the same as that for the corresponding scalar model which for the present case is $\Gamma_2 = 2A_{1g} + F_{1u} + F_{2g} + A_{2u}$. Then we get the result also obtained elsewhere [7] in a different way,

$$\begin{aligned} \Gamma &= \Gamma_1 \otimes \Gamma_2 \\ &= F_{1u} \otimes (2A_{1g} + F_{1u} + F_{2g} + A_{2u}) \\ &= A_{1g} + 3F_{1u} + E_g + 2F_{2g} + A_{2u} + F_{2u} + F_{1g} + E_u \qquad (5.51) \end{aligned}$$

where we have used the results,

$$\begin{aligned} F_{1u} \otimes A_{1g} &= F_{1u} \\ F_{1u} \otimes F_{1u} &= A_{1g} + E_g + F_{1g} + F_{2g} \qquad (5.52) \\ F_{1u} \otimes F_{2g} &= A_{2u} + E_u + F_{1u} + F_{2u} \\ \text{and} \quad F_{1u} \otimes A_{2u} &= F_{2g} \end{aligned}$$

The above equation immediately shows that in the partial wave expansion, we will have S, P, D_1, D_2, F_1, F_2, G and H type of waves where the nomenclature is that depicted in Appendix III.

The sum of D_1 and D_2 waves is the D wave and that of F_1 and F_2 is the F wave. We have distinguished between D_1 and D_2 because they arise due to different irreducible representations of O_h .

The $\hat{V}$ - matrix can be evaluated by using the projection technique described in Appendix III with the aid of equation (5.51) for Γ . An alternative method will be to use the Clebsch - Gordon Co - efficients for the direct products given by equations (5.52) and use the known basis functions for Γ_2 which form the columns of matrix $\hat{V}_B$ given in Appendix III along with the fact that the basis functions for Γ_1 are simply $\begin{bmatrix}1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\end{bmatrix}$ and $\begin{bmatrix}0\\0\\1\end{bmatrix}$.

This method is elegant and useful. The resulting matrix is depicted as $\hat{V}_P$ in Appendix III , the columns of which are eigenvectors of the symmetry types in the following order ,

P , S , D_1, D_2 , F_1 , F_2 , G and H.

The rows are labelled in the same way as those for the matrix $\hat{p}$. In fact $\hat{V}_P$ can be partitioned in the same way as $\hat{p}$ to give ,

$$\hat{V}_P = \begin{bmatrix} \hat{V}_{11} & \hat{V}_{12} & \hat{V}_{13} \\ \hat{V}_{21} & \hat{V}_{22} & \hat{V}_{23} \\ \hat{V}_{31} & \hat{V}_{32} & \hat{V}_{33} \end{bmatrix} \qquad (5.53)$$

and a comparison with $\hat{V}_P$ depicted in Appendix III gives the structure of these 9 x 9 submatrices $\hat{V}_{ij}$.

For example ,

$$\hat{V}_{11} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c & 0 & 0 & 0 & d & 0 & 0 & d \\ 0 & c & 0 & 0 & 0 & -d & 0 & 0 & -d \\ 0 & c & 0 & 0 & 0 & d & 0 & 0 & -d \\ 0 & c & 0 & 0 & 0 & -d & 0 & 0 & d \\ 0 & c & 0 & 0 & 0 & d & 0 & 0 & d \\ 0 & c & 0 & 0 & 0 & -d & 0 & 0 & -d \\ 0 & c & 0 & 0 & 0 & d & 0 & 0 & -d \\ 0 & c & 0 & 0 & 0 & -d & 0 & 0 & d \end{bmatrix} \qquad (5.54)$$

with $c = \frac{1}{\sqrt{8}}$, $d = \frac{1}{\sqrt{16}}$. (5.55)

Similarly one can write down other submatrices.

It has already been pointed out in chapter II that the structure of the block diagonal form of $\hat{p}$, $\hat{g}$, $(\hat{I} + \hat{p}\hat{g})$ and $(\hat{I} + \hat{p}\hat{g})^{-1}$ can be known from the structure of the reducible representation Γ . Thus from the expression for Γ given by equation (5.51) and the order of columns of the matrix $\hat{V}_P$ described, we expect the following block structure given in order.

Three equal 3 x 3 blocks for P- wave.

One single element for S - wave.

Two equal single elements for D_1 - wave.

Three equal 2 x 2 blocks for D_2 - wave.

One single element for F_1 - wave.

Three equal single elements for F_2 - wave.

Three equal single elements for G - wave.

Two equal single elements for H - wave.

The structure of $g_{\alpha\beta}(\omega^2, \underline{R}_n, \underline{R}_n')$ can be written down using equation (5.15) and noting that $e_{\alpha}^{(j)*}(\underline{k})\, e_{\beta}^{(j)}(\underline{k})$ transform like $k_\alpha\, k_\beta$ under inversion and group operations. Also we note that $e_{\alpha}^{(j)*}(\underline{k})\, e_{\beta}^{(j)}(\underline{k})$ is real and if we set

$$\underline{R}_m = \underline{R}_n - \underline{R}'_n \ , \ g_{\alpha\beta}(\omega^2, \underline{R}_n , \underline{R}'_n) = g_{\alpha\beta}(\omega^2, |\underline{R}_m|)$$

This leads to the conclusion, (we suppress ω^2 in the following):

$$g_{\alpha\beta}(\underline{R}_n , \underline{R}'_n) = g_{\beta\alpha}(\underline{R}_n , \underline{R}'_n) \qquad (5.56)$$

and
$$g_{\alpha\beta}(\underline{R}_n , \underline{R}'_n) = g_{\alpha\beta}(\underline{R}'_n , \underline{R}_n) \qquad (5.57)$$

For the model under consideration, $|\underline{R}_m|$ can have five values which appear as subscripts 0 to 4 in the following which in terms of the components read $(0, 0, 0)$, $(\pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$, $(\pm 1, 0, 0)$ and its cyclic permutations, $(\pm 1, \pm 1, 0)$ and its cyclic permutations and $(\pm 1, \pm 1, \pm 1)$. These are the same as those for the scalar model. Inserting these values of $\underline{R}_m$ into the expressions for $g_{\alpha\beta}(\omega^2, |\underline{R}_m|)$ we get the following different Green function elements.

For $g_{\alpha\alpha}(\underline{R}_n , \underline{R}'_n)$, $\alpha = 1, 2, 3$ we have

$$g_{D0} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\ e^{(j)}_{\alpha}(\underline{k})}{\omega^2 - \omega^2_j(\underline{k}) - i\epsilon}$$

$$= \frac{1}{3\,N\,M} \sum_{\underline{k}} \sum_{j} \frac{1}{\omega^2 - \omega^2_j(\underline{k}) - i\epsilon} \qquad (5.58)$$

$$g_{D1} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\ e^{(j)}_{\alpha}(\underline{k}) \cos\frac{1}{2}k_1 \cos\frac{1}{2}k_2 \cos\frac{1}{2}k_3}{\omega^2 - \omega^2_j(\underline{k}) - i\epsilon}$$

$$= \frac{1}{3\,N\,M} \sum_{\underline{k}} \sum_{j} \frac{\cos\frac{1}{2}k_1 \cos\frac{1}{2}k_2 \cos\frac{1}{2}k_3}{\omega^2 - \omega^2_j(\underline{k}) - i\epsilon} \qquad (5.59)$$

$$g_{D4} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\; e^{(j)}_{\alpha}(\underline{k})\; \cos k_1 \cos k_2 \cos k_3}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon}$$

$$= \frac{1}{3\,N\,M} \sum_{\underline{k}} \sum_{j} \frac{\cos k_1 \cos k_2 \cos k_3}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon} \qquad (\;5.60)$$

$$g_{D21} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\; e^{(j)}_{\alpha}(\underline{k})\; \cos k_{\alpha}}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon} \;. \qquad (5.61\;)$$

$$\alpha = 1,2,3$$

$$g_{D22} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\; e^{(j)}_{\alpha}(\underline{k})\; \cos k_{\beta}}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon} \;, \qquad (5.62\;)$$

$$\alpha,\; \beta = 1,2,3\;,\quad \beta \neq \alpha$$

$$g_{D31} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\; e^{(j)}_{\alpha}(\underline{k})\; \cos k_{\alpha} \cos k_{\beta}}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon} \qquad (5.63)$$

for $\alpha, \beta = 1,2,3, \quad \alpha \neq \beta$

and

$$g_{D32} = \frac{1}{NM} \sum_{\underline{k}} \sum_{j} \frac{e^{*(j)}_{\alpha}(\underline{k})\; e^{(j)}_{\alpha}(\underline{k})\; \cos k_{\beta} \cos k_{\beta'}}{\omega^2 - \omega^2_j(\underline{k}) - i\,\epsilon} \;;$$

$$\alpha,\; \beta,\; \beta' = 1,2,3 \qquad (5.64)$$

such that $\alpha \neq \beta, \quad \beta \neq \beta'$

and $\alpha \neq \beta'$.

These are the independent elements occuring in $g_{11}(\underline{R}_n, \underline{R}'_n)$, $g_{22}(\underline{R}_n, \underline{R}'_n)$ and $g_{33}(\underline{R}_n, \underline{R}'_n)$.

For $g_{\alpha\beta}(\underline{R}_n, \underline{R}'_n)$, $\alpha \neq \beta$, $\alpha, \beta = 1,2,3,$ we get

$$g_{N1} = \frac{1}{NM} \sum_{\underline{k}} \sum_{j} \frac{e_{\alpha}^{*(j)}(\underline{k})\, e_{\beta}^{(j)}(\underline{k})\, e^{i(\pm \frac{1}{2}k_1 \pm \frac{1}{2}k_2 \pm \frac{1}{2}k_3)}}{\omega^2 - \omega_j^2(\underline{k}) - i\epsilon} \tag{5.65}$$

$$g_{N4} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e_{\alpha}^{*(j)}(\underline{k})\, e_{\beta}^{(j)}(\underline{k})\, e^{i(\pm k_1 \pm k_2 \pm k_3)}}{\omega^2 - \omega_j^2(\underline{k}) - i\epsilon} \tag{5.66}$$

$$g_{N3} = \frac{1}{N\,M} \sum_{\underline{k}} \sum_{j} \frac{e_{\alpha}^{*(j)}(\underline{k})\, e_{\beta}^{(j)}(\underline{k})\, e^{i(\pm k_\alpha \pm k_\beta)}}{\omega^2 - \omega_j^2(\underline{k}) - i\epsilon} \tag{5.67}$$

The subscripts D and N refer to diagonal and non-diagonal partitions of $\hat{g}$. The first index refers to the $|\underline{R}_m|$ values and the second index refers to the different types arising from the same $|\underline{R}_m|$ value.

With these one can block diagonalize $\hat{g}$ and $\hat{p}$ and hence $(\hat{I} + \hat{p}\hat{g})$ whose inverse can be found and then $\underline{s}_\alpha$ vectors can be calculated.

The resonance denominators are given by,

$$F_S = 1 - \Delta\beta_1 \Big[(g_{D0} - g_{D4}) - (g_{D21} - g_{D31}) + 2(g_{D22} - g_{D32}) - 2(g_{N3} + g_{N4}) \Big] \tag{5.68}$$

$$F_P = \det \left| (I + \hat{\Delta}_p \hat{\Delta}_g) \right| \tag{5.69}$$

where

$$\hat{\Delta}_p = \begin{bmatrix} \Delta M \omega^2 - 8\Delta\beta_1 & 8c\Delta\beta_1 & 16\Delta\beta_2 d \\ 8c\Delta\beta_1 & -\Delta\beta_1 & 0 \\ 16\Delta\beta_2 d & 0 & -\Delta\beta_1 \end{bmatrix}$$

and

$$\hat{\Delta}_g = \begin{bmatrix} g_{D0} & 8c\,g_{D1} & 16d\,g_{N1} \\ 8cg_{D1} & \left[g_{D0} + g_{D4} + g_{D21} + g_{D31} + 2(g_{D22} + g_{D32})\right] & \sqrt{2}(g_{N3} + g_{N4}) \\ 16dg_{N1} & \sqrt{2}(g_{N3} + g_{N4}) & \left[g_{D0} + g_{D4} - g_{D21} - g_{D31} - g_{N3} + g_{N4}\right] \end{bmatrix}$$

where c and d are defined in equation (5.55).

$$F_{D1} = 1 - \Delta\beta_1\left[(g_{D0} - g_{D4}) - (g_{D21} - g_{D31}) + 2(g_{D22} - g_{D32}) + (g_{N3} + g_{N4})\right] \qquad (5.70)$$

$$F_{D2} = \left\{1 - \Delta\beta_1\left[(g_{D0} - g_{D4}) + (g_{D21} - g_{D31}) - (g_{N3} + g_{N4})\right]\right\} \times \left\{1 - \Delta\beta_1\left[(g_{D0} - g_{D4}) - (g_{D21} - g_{D31}) - 2(g_{D22} - g_{D32})\right]\right\} - 2(\Delta\beta_1)^2\,(g_{N3} - g_{N4})^2 \qquad (5.71)$$

$$F_{F1} = 1 - (\Delta\beta_1)\left[(g_{D0} + g_{D4}) + (g_{D21} + g_{D31}) - 2(g_{D22} + g_{D32}) - 2(g_{N3} - g_{N4})\right] \qquad (5.72)$$

$$F_{F2} = 1 - (\Delta\beta_1)\left[(g_{D0} + g_{D4}) - (g_{D21} + g_{D31}) + (g_{N3} - g_{N4})\right] \qquad (5.73)$$

$$F_G = 1 - (\Delta\beta_1)\Big[(g_{D0} - g_{D4}) + (g_{D21} - g_{D31}) + (g_{N3} + g_{N4})\Big] \quad (5.74)$$

and

$$F_H = 1 - (\Delta\beta_1)\Big[(g_{D0} + g_{D4}) + (g_{D21} + g_{D31}) - 2\,(g_{D22} + g_{D32}) + (g_{N3} - g_{N4})\Big] \quad (5.75)$$

An alternative way of finding the $\underline{s}_\nu$ vectors is to use the Clebsch - Gordon Co-efficients and to make use of the results for the scalar model. This is easy to do with the single factor blocks but for bigger blocks the problem of indexing the Green function makes the process complicated.

Once the $\underline{S}_\nu$ vectors are calculated, one can find $F(\underline{k}^i, \underline{k}_o^j)$ appearing in equation (5.50). The expression for $F(\underline{k}^i, \underline{k}_o^j)$ contains contributions from S, P, D_1, D_2, F_1, F_2, G and H type of waves in general. However in the limit of long waves, the F_1, F_2 and H type of waves do not contribute. This can be anticipated by examining the result for the scalar model where in the limit of long waves only the waves corresponding to $2A_{1g} + F_{1u}$ contribute. Hence in the present case one expects to find contributions from waves corresponding to $F_{1u} \otimes (2A_{1g} + F_{1u})$

$$= 2F_{1u} + A_{1g} + E_g + F_{1g} + F_{2g} \quad (5.76)$$

and this leads to precisely those waves that contribute to $F(\underline{k}^i, \underline{k}_o^j)$ in the limit of long waves. Thus in this limit,

$$F(\underline{k}^i, \underline{k}_o^j) = F^{(S)}(\underline{k}^i, \underline{k}_o^j) + F^{(P)}(\underline{k}^i, \underline{k}_o^j) + F^{(D1)}(\underline{k}^i, \underline{k}_o^j) + F^{(D_2)}(\underline{k}^i, \underline{k}_o^j) + F^{(G)}(\underline{k}^i, \underline{k}_o^j) \quad (5.77)$$

where $\underline{k}$ and i specify the wave vector and polarization of the incident phonons and $\underline{k}_o^j$ and j specify those for the scattered phonons when $\underline{k}_o^j$ lie along symmetry directions. Using the long - wavelength limit expression for incidence along (100) direction,

$$g_\beta(\underline{k}_o^j) = \frac{e_\beta^{(j)*}(\underline{k}_o^j)}{\pi \times 8\beta_1} = \frac{e_\beta^{(j)*}(\underline{k}_o^j)}{\pi M \omega_o^2}$$

$$\text{with } \omega_o^2 = \frac{8\beta_1}{M} \tag{5.78}$$

the expressions for $F^{(\nu)}(\underline{k}^i, \underline{k}_o^j)$ are found to be

$$F^{(S)}(\underline{k}^i, \underline{k}_o^j) = -\left(\frac{1}{3\pi F_S}\right)\left(\frac{\Delta\beta_1}{\beta_1}\right)\left[\sum_\ell k_\ell e^{(i)}(\underline{k})\right] \times \left[\sum_{\ell'} \underline{k}^j_{o\ell'} \overset{*}{e}{}^{(j)}_{\ell'}(\underline{k}_o^j)\right] \tag{5.79}$$

$$F^{(p)}(\underline{k}^i, \underline{k}_o^j) = \left(\frac{1}{\pi M \omega_o^2 F_p}\right)(h_1 + 8h_2)\left(\sum_\ell e_\ell^{(i)}(\underline{k})\ \overset{*}{e}{}_\ell^{(j)}(\underline{k}_o^j)\right) \tag{5.80}$$

with

$$h_1 = \Delta M\omega^2\left[\Delta_{22}\Delta_{33} - \Delta_{23}\Delta_{32}\right] + \sqrt{16}\,\Delta\beta_2 \times \left[\Delta_{12}\Delta_{23} - \Delta_{22}\Delta_{13}\right] \tag{5.81}$$

$$h_2 = \frac{\Delta M\omega^2}{\sqrt{8}}\left[\Delta_{23}\Delta_{31} - \Delta_{21}\Delta_{33}\right] + \sqrt{2}\,\Delta\beta_2 \times \left[\Delta_{21}\Delta_{13} - \Delta_{23}\Delta_{11}\right] \tag{5.82}$$

where $\hat{\Delta} = \hat{I} + \hat{\Delta}_p \hat{\Delta}_g$, the 3 x 3 matrices $\hat{\Delta}_p$ and $\hat{\Delta}_g$ are defined after equation (5.69).

$$F^{(D_1)}(\underline{k}^i,\underline{k}_o^j) = \left(-\frac{1}{2\pi F_{D_1}}\right)\left(\frac{\Delta\beta_1}{\beta_1}\right)\Big[\left\{k_1\, e_1^{(i)}(\underline{k}) - k_2\, e_2^{(i)}(\underline{k})\right\}$$

$$\times\left\{k_{o1}\, e_1^{*(j)}(\underline{k}_o^j) - k_{o2}\, e_2^{*(j)}(\underline{k}_o^j)\right\} + \frac{1}{3}\left\{k_1\, e_1^{(i)}(\underline{k}) + k_2\, e_2^{(i)}(\underline{k}) - 2k_3 e_3^{(i)}(\underline{k})\right\}$$

$$\times\left\{k_{o1}\, e_1^{*(j)}(\underline{k}_o^j) + k_{o2}\, e_2^{*(j)}(\underline{k}_o^j) - 2k_{o3}\, e_3^{*(j)}(\underline{k}_o^j)\right\} \qquad (5.83)$$

$$F^{(D_2)}(\underline{k}^i,\underline{k}_o^j) = \left(-\frac{1}{2\pi F_{D2}}\right)\left(\frac{\Delta\beta_1}{\beta_1}\right)\left(1 - \Delta\beta_1\lambda_4\right)$$

$$\times\Big[\left\{k_2\, e_1^{(i)}(\underline{k}) + k_1\, e_2^{(i)}(\underline{k})\right\}\left\{k_{o2}\, e_1^{*(j)}(\underline{k}_o^j) + k_{o1}\, e_2^{*(j)}(\underline{k}_o^j)\right\}$$

$$+\left\{k_3\, e_1^{(i)}(\underline{k}) + k_1\, e_3^{(i)}(\underline{k})\right\}\left\{k_{o3}\, e_1^{*(j)}(\underline{k}_o^j) + k_{o1}\, e_3^{*(j)}(\underline{k}_o^j)\right\}$$

$$+\left\{k_3\, e_2^{(i)}(\underline{k}) + k_2\, e_3^{(i)}(\underline{k})\right\}\left\{k_{o3} e_2^{*(j)}(\underline{k}_o^j) + k_{o2}\, e_3^{*(j)}(\underline{k}_o^j)\right\}\Big] \qquad (5.84)$$

where

$$\lambda_4 = (g_{D0} - g_{D4}) - (g_{D21} - g_{D31}) - 2(g_{D22} - g_{D32})$$

and

$$F^{(G)}(\underline{k}^i,\underline{k}_o^j) = \left(-\frac{1}{2\pi F_G}\right)\left(\frac{\Delta\beta_1}{\beta_1}\right)\Big[\left\{k_2 e_3^{(i)}(\underline{k}) - k_3 e_2^{(i)}(\underline{k})\right\} \times \qquad (5.85)$$

$$\left\{k_{o2}\, e_3^{*(j)}(\underline{k}_o^j) - k_{o3}\, e_2^{*(j)}(\underline{k}_o^j)\right\} + \left\{k_3\, e_1^{(i)}(\underline{k}) - k_1\, e_3^{(i)}(\underline{k})\right\}$$

$$\times\left\{k_{o3}\, e_1^{*(j)}(\underline{k}_o^j) - k_{o1}\, e_3^{*(j)}(\underline{k}_o^j)\right\} + \left\{k_1 e_2^{(i)}(\underline{k}) - k_2 e_1^{(i)}(\underline{k})\right\}$$

$$\times\left\{k_{o1}\, e_2^{*(j)}(\underline{k}_o^j) - k_{o2}\, e_1^{*(j)}(\underline{k}_o^j)\right\}\Big] \qquad (5.86)$$

In all the equations above one must evaluate the quantities

F_S , F_P , F_{D1} , F_{D2} , and F_G in the long wave length limit.

Let the (incident) phonons be incident along the (100) direction. Then $k_1 = k, k_2 = 0 , k_3 = 0$ and the total scattering cross section is given by the optical theorem.

$$\sigma_T = \frac{4\pi}{k} \text{Im} \left[F(\underline{k}^i, \underline{k}^i) \right] \tag{5.87}$$

(i) Longitudinal polarization :- Here $e_\beta^{(i)}(\underline{k}) = \delta_{\beta 1}$. Now $F(\underline{k}^i, \underline{k}^i)$ with $\underline{k}$ and i specified as above leads to the following partial wave contributions,

$$F^{(S)}(\underline{k}^i , \underline{k}^i) = - \frac{k^2}{3\pi F_S} , \quad F^{(P)} = \frac{1}{\pi M\omega_o^2 F_P} (h_1 + 8h_2)$$

$$F^{(D1)} = - \frac{2 k^2}{3\pi F_{D1}} \tag{5.88}$$

$$F^{(D_2)} = 0 = F^{(G)}$$

(ii) Transverse polarisation :- Here $e_\beta^{(i)}(\underline{k}) = \delta_{\beta 2}$ or $\delta_{\beta 3}$

$$F^{(S)} = 0 = F(D_1)$$

$$F^{(P)} = \frac{1}{\pi M\omega_o^2 F_P} (h_1 + 8h_2)$$

$$F^{(D_2)} = \left(- \frac{1}{2\pi F_{D2}} \right) \left(\frac{\Delta\beta_1}{\beta_1} \right) (1-\Delta\beta_1 \lambda_4) k^2$$

$$F^{(G)} = \left(- \frac{1}{2\pi F_G} \right) \left(\frac{\Delta\beta_1}{\beta_1} \right) k^2 \tag{5.89}$$

Now we have for the Green functions in the limit of long waves

$$\text{Im } g_{D0} = x_1 , \quad \text{Im } g_{D1} = x_1 + \frac{x_2 b_2}{48} , \quad \text{Im } g_{D4} = \cancel{x_1} + \frac{x_2 b_2}{12} \tag{5.90}$$

with $$b_2 = \sum_j \int \frac{\sin\theta \, d\theta \, d\varphi}{\left[F_j(\theta, \varphi) \right]^{5/2}} \qquad (5.91)$$

where $F_j(\theta, \varphi)$ is given by équation (5.35).

$$\mathrm{Im}\ g_{D21} = (x_1 + x_2 b_3), \quad \mathrm{Im}\ g_{D31} = (x_1 + x_2 b_5)$$
$$\mathrm{Im}\ g_{D22} = (x_1 + x_2 b_4), \quad \mathrm{Im}\ g_{D32} = (x_1 + x_2 b_6) \qquad (5.92)$$
$$\mathrm{Im}\ g_{N1} = x_2 b_7, \quad \mathrm{Im}\ g_{N2} = 4x_2 b_7, \quad \mathrm{Im}\ g_{N3} = x_2 b_8$$

where $$x_1 = -\frac{\omega \pi \ b_1}{6 M V^* \omega_o^3}, \quad x_2 = \frac{\pi \omega^3}{M V^* \omega_o^5},$$

and b_i, $i = 3$ to 8, are cumbersome integrals over angles like b_1 and b_2 described in equations (5.35) and (5.91). These yield numerical values after integration with given ratios of $\left(\frac{\beta_2}{\beta_1} \right)$.

Using all these results and the optical theorem along with the fact that for (100) direction of incidence, $k^2 = \frac{8\omega^2}{\omega_o^2}$, one gets the results,

$$\sigma_T^{(100)L} = \left(\frac{\omega}{\omega_o}\right)^4 \Bigg[\left(\frac{\Delta\beta_1}{\beta_1}\right)^2 \left\{ \frac{a_1}{|F_S|^2} + \frac{a_2}{|F_{1}|^2} \right\}$$
$$+ \frac{1}{|F_P|^2} \left(\frac{\Delta M}{M}\right)^2 \left\{ a_3 + \left(a_4 + a_5 \frac{\Delta\beta_1}{\beta_1}\right)^2 + \left(a_6 + a_7 \frac{\Delta\beta_2}{\beta_2}\right)^2 \right.$$
$$\left. + a_8 \left(\frac{\Delta\beta_1}{\beta_1}\right) \left(\frac{\Delta\beta_2}{\beta_2}\right) \right\} \Bigg] \qquad (5.93)$$

and

$$\sigma_T^{(100)T} = \left(\frac{\omega}{\omega_o}\right)^4 \Bigg[\left(\frac{\Delta\beta_1}{\beta_1}\right)^2 \left\{ \frac{a_9}{|F_{D2}|^2} + \frac{a_{10}}{|F_G|^2} \right\} \ldots$$

$$+ \frac{1}{|F_p|^2} \left(\frac{\Delta M}{M}\right)^2 \left\{ a_3 + \left(a_4 + a_5 \frac{\Delta \beta_1}{\beta_1}\right)^2 + \left(a_6 + a_7 \frac{\Delta \beta_2}{\beta_2}\right)^2 + a_8 \left(\frac{\Delta \beta_1}{\beta_1}\right)\left(\frac{\Delta \beta_2}{\beta_2}\right) \right\} \Bigg] \tag{5.94c}$$

Here T and L refer to the transverse and longitudinal polarizations respectively and the numerical quantities a_i, $i = 1, \dots, 10$ are appropriate combinations of b_i, $i = 1, \dots, 8$ and other numerical factors.

Similar expressions can be derived for other incident directions and polarisations. However the partial waves contributing for different incident directions and polarizations are different. Table II below gives the result in the limit of long waves.

TABLE II

Direction of Incidence.	Polarisation	Normalized Polarization vectors (transpose)	Partial waves contributing to σ_T	Partial waves interferingin the expression for $\Lambda^{-1}(\omega)$	Remarks
100	Longitudinal	(1 0 0)	S, P, D_1	S-P, P-D_1	The two transverse branches are degenerate
	Transverse	(0 1 0)	P, D_2, G	P-D_2, P-G	
	Transverse	(0 0 1)	P, D_2, G	P-D_2, P-G	
110	Longitudinal	$\frac{1}{\sqrt{2}}$(1 1 0)	S, P, D_2	S-P, P-D_2	Transverse branches are non-degenerate
	Transverse	(0 0 1)	P, D_2, G	P-D_2, P-G	
	Transverse	$\frac{1}{\sqrt{2}}$(1 -1 0)	P, D_1, G	P-D_1, P-G	
111	Longitudinal	$\frac{1}{\sqrt{3}}$(1 1 1)	S, P, D_2	S-P, P-D_2	Transverse branches are degenerate
	Transverse	$\frac{1}{\sqrt{2}}$(1 -1 0)	P, D_1, D_2, G	P-D_1, P-D_2, P-G	
	Transverse	$\frac{1}{\sqrt{6}}$(1 1 -2)	P, D_1, D_2, G	P-D_1, P-D_2, P-G	

It should be noted that even in the limit of long waves, the number of partial waves contributing to the total cross section depends upon the direction of incidence. This feature is a consequence of the significant departure of long wave behavior in the present model from the usual Debye approximation. It is in fact related to the behavior of the dispersion which in the limit of small $\underline{k}$ becomes,

$$\omega_j^2(\underline{k}) = \frac{\beta_1 k^2}{M} - \frac{8\beta_2}{2M}\sqrt{\left\{(k_1^2 k_2^2 + k_2^2 k_3^2 + k_3^2 k_1^2)/3\right\}}\cos\left(\frac{\lambda}{3} + \frac{2\pi j}{3}\right) \tag{5.95}$$

for $j = 1,2,3$

with

$$\cos^2\lambda = \frac{27\,(k_1^2 k_2^2 k_3^2)^2}{(k_1^2 k_2^2 + k_2^2 k_3^2 + k_3^2 k_1^2)^3} \tag{5.96}$$

This shows that the constant frequency surfaces in this long wavelength limit are not spheres as would be the case if Debye model is assumed. Although this departure showed itself up for the case of isotope defect in the numerical factor as seen already, it affects the case of a general substitutional impurity quite significantly. For example the inverse mean free path will contain interference terms between different partial wave contributions depending upon the direction of incidence and the polarization of the incident phonons. This is shown in the above table. It is to be noted that interference occurs between waves of different 'parities'.

From the expressions for the total cross-section one finds that the change of mass affects only the P wave contribution whereas the change in force constants affects all the waves. The low energy and hence long wavelength scattering shows the expected Rayleigh type of scattering in absence of resonances. However the presence of resonance denominators include the possibility of resonance scattering. A comparison of the results obtained here with those of the scalar model discussed in the last chapter shows that there is a change in 'parity' of the waves in the two models. For example the, S - wave of the scalar model goes over to the P - wave in this case and so on. This result is expected by simple group theoretical arguments.

5.5 Summary :

In this chapter the model considered may be claimed to be a step forward in the approximation to the realistic case, compared to those considered in the last two chapters. As expected one gets some results that are qualitatively the same as those for the scalar model. Among these are the modified Rayleigh type of scattering at low frequencies with resonance possibility and the interference between waves of different 'parities ' in the expression for $\Lambda^{-1}(\omega)$. One of the differences lies in the consequences related to the validity of Debye approximation in the long wavelength limit and the shape of the constant frequency surfaces in this limit. It turns out that in this limit the constant frequency surfaces are not spheres in general and hence Debye approximation does not hold. However it is remarkable that for the isotope case this leads to the same result as that obtained by using Debye approximation except for a numerical factor which depends upon the direction of incidence. For the case of a general substitutional impurity it has the effect of making the long wavelength total cross - section dependent upon the incident direction unlike the scalar model where it becomes independent of incident direction.

We have also discussed how one can go over to the scalar model from the model under consideration by adjusting the force constants suitably.

The other new feature here is of course the dependence of the scattering process on the polarization of incident phonons. It is already apparent that introduction of polarization leads to a great deal of mathematical complexity in the problem. The scattering process becomes quite involved physically also. Compared to the scalar model, the corresponding partial waves appear, as expected, to have changed their 'parities' . Perhaps one can safely contend that these additional features must be present in a realistic case.

CHAPTER VI

CONCLUSION

The results obtained in the present study can be summarized as follows.

The scattering cross section and the number of partial waves contributing to it depend upon the direction of incidence of phonons, thus exhibiting the expected non-central nature of the 'potential' due to a substitutional impurity in a lattice (Chapter IV, Table I).

The resonances in the partial wave amplitudes and the behavior of the scattering cross sections near resonances have been investigated in detail. The results confirm those obtained by other workers. The scattering of both the acoustic and optical phonons in a diatomic simple cubic lattice has been studied and expressions for resonance denominators are obtained explicitly.

The expressions for mean free paths of phonons due to scattering from substitutional impurities have been obtained for small concentration of impurities and phonons with long wavelengths. These expressions are shown to contain interference terms between waves of different 'parities'. Their behavior near resonances has been studied. The similarity of results for the three cubic lattices has been discussed.

The effect of polarization of phonons on the scattering process has been studied by using a suitable model of body centred cubic lattice in Chapter V. It has been pointed out that the results obtained for this case can be taken over to the case of the so called scalar models by an appropriate choice of force constants. The Debye model is shown to be inadequate for the exact description of the scattering process in the limit of long waves. The departure from the Debye model in this limit leads to the dependence of the scattering process on the direction of incidence (Chapter V, Table II).

The entire study has been based upon the harmonic approximation and nearest neighbour interaction models. The effect of anharmonicity on the phonons in the impure crystal is rather complicated, and leads to a finite life-time for each phonon.[50] This would affect the phonon mean free path, and the transport coefficients which depend on it. The present analysis is valid at very low temperatures when the anharmonic effects are small, and would be adequate to cover such phenomena as the kinks in thermal conductivity curves obtained by many workers[22-23,25-26].

The other essential limitation of the models investigated here is that the impurity is taken as a substitutional one. There is enough experimental evidence now[51] to indicate that quite often the impurity atom (or molecule) goes into interstitial positions. The symmetry of the impurity 'potential' in such cases is surely more complicated than what has been assumed in the present analysis. A proper theory of phonon scattering from impurities must take such situations into account.

APPENDIX I

GREEN FUNCTIONS FOR SCALAR MODELS

The elements of the Green function matrix for a scalar model are of the form,

$$G(\omega^2, \underline{R}_i, \underline{R}_j) = -\frac{1}{MV^*}\iiint \frac{\exp\left[i\underline{k}.(\underline{R}_i-\underline{R}_j)\right] d^3k}{\omega^2(\underline{k}) - \omega^2 - i\epsilon} \qquad \text{(AI-1)}$$

where $\omega^2(\underline{k})$ is the appropriate dispersion, the components of $\underline{R}_i$ and $\underline{R}_j$ are measured in the units of the corresponding lattice spacings. Then $\underline{k}$ is dimensionless wave vector and the $\underline{k}$ integration is over the first Brillouin zone whose volume is V^*. For the simple cubic lattice $\underline{k}$ integrations extend from $-\pi$ to $+\pi$ with $V^* = (2\pi)^3$, the unit of measurement being the lattice spacing a^{-1}.

For face centred cubic and body centred cubic lattices the symmetry of the constant frequency surfaces can be exploited by doing the integration through 1/48 of the Brillouin zone[48], which in the face centred cubic case is the part of the zone enclosed in the trihedral angle defined by (001), (101) and (111) directions; and in the body centred cubic case is the part enclosed within the tetrahedron bounded by the planes $k_2 = 0$, $k_1 + k_3 = \pi$, $k_1 = k_2$ and $k_1 = k_3$ with their ranges defined by $0 \leqslant k_1, k_2 \leqslant \frac{\pi}{2}$ and $0 \leqslant k_3 \leqslant \pi$. It is also possible to combine these wedges to form a cube in the reciprocal space whose sides are of length 4π i.e. from -2π to $+2\pi$ such that integration over this cube gives four times the result of integration over the Brillouinzone for the body centred cubic lattice and twice the result of integration over the Brillouin zone for the face centred cubic lattice. We choose this cube for integration because of the analytic convenience it offers for body centred cubic and face centred cubic lattices. With this choice and a change of variable one obtains

$$G_{B,F}(\omega^2, \underline{R}_i, \underline{R}_j) = \frac{-1}{M(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{\exp\left[2i\underline{k}.(\underline{R}_i-\underline{R}_j)\right] d^3k}{\omega^2_{B,F}(2\underline{k}) - \omega^2 - i\epsilon}$$

(AI-2)

whereas for the simple cubic lattice

$$G_S(\omega^2, \underline{R}_i, \underline{R}_j) = \frac{-1}{M(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{\exp\left[i\underline{k}.(\underline{R}_i-\underline{R}_j)\right] d^3k}{\omega^2_S(\underline{k}) - \omega^2 - i\epsilon}$$

(AI-3)

The subscripts S, B and F refer to simple cubic, body centred cubic and face centred cubic lattices respectively. The asymptotic expansion is obtained from equation (AI-1) for large $R = |\underline{R}_i-\underline{R}_j|$, and this is discussed in Appendix II. Since $G(\omega^2, \underline{R}_i, \underline{R}_j)$ depends upon $|\underline{R}_i-\underline{R}_j|$, in what follows, we shall adopt the convention of writing the Cartesian components of $\underline{R}_i-\underline{R}_j$ in the units of the lattice constant 'a' of these cubic lattices. Thus for example $G_B(\omega^2, 1,1,0)$ stands for $\underline{R}_i-\underline{R}_j = a\underline{e}_1 + a\underline{e}_2$ in body centred cubic lattice, $G_F(\omega^2, 1, \frac{1}{2}, \frac{1}{2})$ stands for $\underline{R}_i-\underline{R}_j = a(\underline{e}_1 + \frac{1}{2}\underline{e}_2 + \frac{1}{2}\underline{e}_3)$ in face centred cubic lattice and so on. Here $\underline{e}_i$ are the unit vectors along the Cartesian axes.

The Green functions which occur in the expressions for the scattering amplitudes are conveniently evaluated in terms of the parameters $E_S = 3 - \frac{\omega^2}{\omega_{oS}^2}$, $E_B = 1 - \frac{\omega^2}{\omega_{oB}^2}$ and $E_F = 3 - \frac{\omega^2}{\omega_{oF}^2}$, so that the frequency bands are defined by the ranges $-3 \leqslant E_S \leqslant 3$, $-1 \leqslant E_B \leqslant 1$ and $-1 \leqslant E_F \leqslant 3$ respectively. These E_S, E_B and E_F are dimensionless energy parameters.

For the simple cubic lattice, the Green function elements occuring in the expressions for the scattering amplitudes can be derived from the general expression

$$G(p,q,r,E_S) = \lambda_S \left[\frac{1}{(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{d^3k \cos pk_1 \cos qk_2 \cos rk_3}{E_S - \cos k_1 - \cos k_2 - \cos k_3 - i\epsilon} \right] \tag{AI-4}$$

where $\lambda_S = -1/(M\omega_{oS}^2) = -1/(2\Upsilon)$. The integral inside the paranthesis can be written[28] as.

$$I(p,q,r,E_s) = i^{p+q+r+1} \left[C(p,q,r,E_s) - i\, S(p,q,r,E_s) \right] \tag{AI-5}$$

with

$$C(p,q,r,E_s) = \int_0^\infty dx \cos(E_s x)\, J_p(x)\, J_q(x)\, J_r(x) \tag{AI-6}$$

and

$$S(p,q,r,E_s) = \int_0^\infty dx \sin(E_s x)\, J_p(x)\, J_q(x)\, J_r(x) \tag{AI-7}$$

Here $J_p(x)$ is the Bessel function of first kind of order p. The numerical values of the functions $C(p,q,r,E_s)$ and $S(p,q,r,E_s)$ for the (p,q,r) values of (0,0,0), (1,0,0), (1,1,0) and (2,0,0) have been tabulated extensively[28,32]. In the limit of long waves one gets

$$\mathrm{Im}\, I(p,q,r,E_s) = \frac{\omega}{\sqrt{2}\,\pi\,\omega_{oS}} - \frac{\omega^3}{3\sqrt{2}\,\pi\,\omega_{oS}^3}(p^2+q^2+r^2) \tag{AI-8}$$

where we have employed the following method.

If $F_1(\underline{k})$ and $F_2(\underline{k})$ are two functions of $\underline{k}$, then we can write the integral

$$I = \mathrm{Im}\int \frac{d^3k\, F_2(\underline{k})}{F_1(\underline{k}) - i\epsilon} = \pi \int d^3k\, F_2(\underline{k})\, \delta(F_1(\underline{k})) \tag{AI-9}$$

using the formula $\dfrac{1}{x - i\epsilon} = \dfrac{P}{x} + i\pi\,\delta(x)$.

Now we can further write

$$I = \pi \int \frac{dS\, F_2(\underline{k})}{|\nabla_k F_1(\underline{k})|} \tag{AI-10}$$

where the integration is over the surface of constant $\underline{k}$ where $\underline{k}$ is the solution of $F_1(\underline{k}) = 0$. All these are evaluated at the limit of long waves. Explicitly one has

$$C(0,0,0,E_s) = \frac{\omega}{\sqrt{2}\,\pi\,\omega_{oS}} \tag{AI-11a}$$

$$S(1,0,0,E_s) = \frac{\omega}{\sqrt{2}\,\pi\,\omega_{oS}} - \frac{\omega^3}{3\sqrt{2}\,\pi\,\omega_{oS}^3} \tag{AI-11b}$$

$$C(1,1,0,E_s) = -\frac{\omega}{\sqrt{2}\,\pi\,\omega_{oS}} + \frac{2\,\omega^3}{3\sqrt{2}\,\pi\,\omega_{oS}^3} \tag{AI-11c}$$

$$C(2,0,0,E_s) = -\frac{\omega}{\sqrt{2}\,\pi\,\omega_{oS}} + \frac{2\sqrt{2}\,\omega^3}{3\,\pi\,\omega_{oS}^3} \tag{AI-11d}$$

For the body centred cubic lattice, the Green functions used in the resonance denominators are

$$G_B(\omega^2, 0,0,0) = g_{oB} = \lambda_B \left[\frac{1}{(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{d^3k}{E_B - \cos k_1 \cos k_2 \cos k_3 - i\epsilon} \right]$$

$$= 2\lambda_B \int_0^\infty dx \; J_o^2(x) \left[J_o(2E_B x) - i\, Y_o(2E_B x) \right]$$

$$= 2\lambda_B \left[GBR_1 - i\, GBI_1 \right] \qquad \text{(AI-12)}$$

$$G_B(\omega^2, \tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) = g_{1B} = E_B\, g_{oB} - \lambda_B \qquad \text{(AI-13)}$$

$$G_B(\omega^2, 1,0,0) = g_{2B} = \lambda_B \left[\frac{1}{(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{d^3k \cos 2k_1}{E_B - \cos k_1 \cos k_2 \cos k_3 - i\epsilon} \right]$$

$$= -2\lambda_B \int_0^\infty dx \; J_1^2(x) \left[J_o(2E_B x) - i\, Y(2E_B x) \right]$$

$$= -2\lambda_B \left[GBR_2 - i\, GBI_2 \right] \qquad \text{(AI-14)}$$

$$G_B(\omega^2, 1,1,0) = g_{3B} = \lambda_B \left[\frac{1}{(2\pi)^3} \iiint_{-\pi}^{+\pi} \frac{d^3k \cos 2k_1 \cos 2k_2}{E_B - \cos k_1 \cos k_2 \cos k_3 - i\epsilon} \right]$$

$$= -2\lambda_B \int_0^\infty dx \; J_o(x)\, J_2(x) \left[J_o(2E_B x) - i\, Y_o(2E_B x) \right]$$

$$= -2\lambda_B \left[GBR_3 - i\, GBI_3 \right] \qquad \text{(AI-15)}$$

$$G_B(\omega^2, 1,1,1) = g_{4B} = 8\, E_B^2 g_{oB} - 8\, E_B \lambda_B - g_{oB} - 3g_{2B} - 3g_{3B}$$

$$= 2\lambda_B \left[GBR_4 - i\, GBI_4 \right] \qquad \text{(AI-16)}$$

where $\lambda_B = -1/M\,\omega^2_{oB} = -1/8\gamma$. J and Y are Bessel functions of first and second kind. The quantities GBR_1 and GBI_i defined above have been computed and their numerical values are available[33]. The distribution function of the frequency (squared) for the body centred cubic lattice, which equals GBI_1 except for a numerical factor, has a logarithmic singularity in the middle of the band in this scalar model.

In the low frequency (long wavelength) limit one can follow the method indicated in equations (AI-9) and (AI-10) to get

$$\text{Im } g_{oB} = \lambda_B\, a_{1B},\ \text{Im } g_{1B} = \lambda_B\,(a_{1B} - a_{2B}),\ \text{Im } g_{2B} = \lambda_B(a_{1B} - \tfrac{4}{3}\, a_{2B})$$

$$\text{Im } g_{3B} = \lambda_B(a_{1B} - \tfrac{8}{3}\, a_{2B}),\ \text{Im } g_{4B} = \lambda_B(a_{1B} - 4a_{2B}) \qquad \text{(AI-17)}$$

with $a_{1B} = 2\sqrt{2}\,\omega/\pi\omega_{oB}$, $a_{2B} = 2\sqrt{2}\,\omega^3/\pi\omega^2_{oB}$ and $1 = 2\sqrt{2}\,\omega/\omega_{oB}$

These are used in the derivation of the long wavelength limit of the scattering amplitudes.

Similarly, for the face centred cubic lattice one obtains,

$$G_F(\omega^2,0,0,0) = g_{oF} = \lambda_F\left[\frac{4}{(2\pi)^3}\iiint_{-\pi}^{+\pi}\frac{d^3k}{E_F-(\cos k_1\cos k_2+\cos k_3\cos k_1 + \cos k_2\cos k_3) - i\epsilon}\right]$$

(AI-18)

$$G_F(\omega^2,\tfrac{1}{2},\tfrac{1}{2},0) = g_{1F} = \tfrac{1}{3}(E_F g_{oF} - 4\,\lambda_F) \qquad \text{(AI-19)}$$

$$G_F(\omega^2,1,0,0) = g_{2F} = \lambda_F\left[\frac{4}{(2\pi)^3}\iiint_{-\pi}^{+\pi}\frac{d^3k\,\cos 2k_1}{E_F-(\cos k_1\cos k_2+\cos k_2\cos k_3 + \cos k_3\cos k_1) - i\epsilon}\right]$$

(AI-20)

$$G_F(\omega^2,1,\tfrac{1}{2},\tfrac{1}{2}) = g_{4F} = \lambda_F\left[\frac{4}{(2\pi)^3}\iiint_{-\pi}^{+\pi}\frac{d^3k\,\cos k_1\cos k_2\cos 2k_3}{E_F-(\cos k_1\cos k_2+\cos k_2\cos k_3+\cos k_3\cos k_1)-i\epsilon}\right] \qquad \text{(AI-21)}$$

and,

$$G_F(\omega^2,1,1,0) = g_{5F} = \lambda_F\left[\frac{4}{(2\pi)^3}\iiint_{-\pi}^{+\pi}\frac{d^3k\,\cos 2k_1\,\cos 2k_2}{E_F-(\cos k_1\cos k_2+\cos k_2\cos k_3+\cos k_3\cos k_1)-i\epsilon}\right] \qquad \text{(AI-22)}$$

where $\lambda_F = -1/4M\,\omega_{oF}^2 = -1/16\gamma$. The long wavelength limit for these are;

$$\mathrm{Im}\,g_{oF} = 4\lambda_F a_{1F},\ \mathrm{Im}\,g_{1F} = 4\lambda_F(a_{1F}-a_{2F}),\ \mathrm{Im}\,g_{2F} = 4\lambda_F(a_{1F}-2a_{2F})$$

$$\mathrm{Im}\,g_{3F} = 4\lambda_F(a_{1F}-a_{2F}),\ \mathrm{Im}\,g_{4F} = 4\lambda_F(a_{1F}-3a_{2F}),\ \mathrm{Im}\,g_{5F} = 4\lambda_F(a_{1F}-4a_{2F}) \qquad \text{(AI-23)}$$

where

$$a_{1F} = \omega/2\pi\omega_{oF},\ a_{2F} = \omega^3/6\pi\omega_{oF}^3 \text{ and } k = 2\,\omega/\omega_{oF}$$

As mentioned above, tables with numerical values of the integrals are available. The numerical computations of these from the forms given above happen to be quite tedious and time consuming. Recently Mahanty[34] has suggested the use of the method of Fourier series expansion of the Green function. This simple technique is based on expanding

$$\mathrm{Im}\, G(\underline{R}, x) = \sum_n a_n(\underline{R}) \sin(n\pi x) \qquad \text{(AI-24)}$$

with $$a_n(\underline{R}) = \frac{2\pi}{V^*} \int_{V^*} d^3k \exp(i\underline{k}.\underline{R}) \sin\left(n\pi E(\underline{k})\right) \qquad \text{(AI-25)}$$

where $E(\underline{k}) = M\omega^2(\underline{k})$ and x is dimensionless energy such that the band is always defined as $0 \leqslant x \leqslant 1$. The real part of $G(\underline{R}, x)$ is given by

$$\mathrm{Re}\, G(\underline{R}, x) = \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\mathrm{Im}\, G(\underline{R}, x')\, dx'}{x' - x} \qquad \text{(AI-26)}$$

The use of this method leads to considerable saving of computational time. It may be noted that the quantities numerically computed do not involve mass or force constants so that these very integrals can also be used for Green functions encountered in the problem of scattering of spin waves and band electrons from a substitutional impurity.

APPENDIX II

ASYMPTOTIC EXPANSION OF GREEN FUNCTION INTEGRALS

A typical Green function integral can be written as

$$G_{\mu\nu}(\omega^2, \underline{R}_i-\underline{R}_j) = G_{\mu\nu}(\omega^2, \underline{R}) = \sum_j G^j_{\mu\nu}(\omega^2, \underline{R}) \qquad \text{(AII-1)}$$

where

$$G^j_{\mu\nu}(\omega^2, \underline{R}) = -\frac{1}{MV^*}\iiint \frac{d^3k\left[\lambda_{\mu\nu}(\underline{k}) \exp(i\underline{k}.\underline{R})\right]}{\omega_j^2(\underline{k}) - \omega^2 - i\epsilon} \qquad \text{(AII-2)}$$

Here $\lambda_{\mu\nu}(\underline{k})$ is some function of $\underline{k}$ which does not involve $\underline{R}$ and $\omega_j^2(\underline{k})$ is a branch of the dispersion. The index j denoting the branch of the dispersion is to be omitted for scalar models. The integration is over the first Brillouin zone and $\epsilon \rightarrow 0$ in the limit. For large R = $|\underline{R}|$ the integral can be expanded by the method of stationary phase which has been discussed by Koster[21] and subsequently used by many authors[9,7,45,13]. The expansion given below is a version of this method suitable for our purpose.

Using the formula

$$\frac{1}{x - i\epsilon} = i\int_0^\infty \exp\left[-i\,(x-i\epsilon)\,t\right] dt$$

equation (AII-2) can be written as

$$G^j_{\mu\nu}(\omega^2, \underline{R}) = -\frac{1}{MV^*}\, I\,(\underline{R}, \omega) \qquad \text{(AII-3)}$$

where $$I\,(\underline{R}, \omega) = i\int_0^\infty dt \iiint d^3k\; \lambda_{\mu\nu}(\underline{k}) \exp\left\{-i\,\varphi\,(\underline{k},t)\right\} \qquad \text{(AII-4)}$$

with the phase $$\varphi\,(\underline{k},t) = \left\{\omega_j^2(\underline{k}) - \omega^2\right\} t - \underline{k}.\underline{R} \qquad \text{(AII-5)}$$

When φ is stationary with respect to $\underline{k}$ and t one has $\frac{\partial\varphi}{\partial t} = 0$ and $\nabla_k \varphi = 0$. These two equations determine at least one $(\underline{k}_o^j, t_o)$ which specify the stationary point. Using (AII-5) one finds that $\underline{k}_o^j$ and t_o are such that

$$\omega_j^2(\underline{k}_o^j) = \omega^2$$

and

$$\nabla_k \omega_j^2(\underline{k}) \Big|_{\underline{k} = \underline{k}_o^j} = \underline{R} / t_o \qquad \text{(AII-6)}$$

Now one can expand $\varphi(\underline{k}, t)$ about this stationary point $(\underline{k}_o^j, t_o)$ by putting $\underline{k} = \underline{k}_o^j + \underline{K}$ and $t = t_o + \tau$ so that

$$\varphi(\underline{k}, t) = -\underline{k}_o^j \cdot \underline{R} + \tau \sum_i \beta_i K_i + t_o \sum_{ij} K_i \alpha_{ij} K_j \qquad \text{(AII-7)}$$

neglecting higher order terms

Here
$$\beta_i = \frac{\partial}{\partial k_i} \omega_j^2(\underline{k}) \Big|_{\underline{k} = \underline{k}_o^j} \qquad \text{(AII-8)}$$

and
$$\alpha_{ij} = \frac{1}{2} \frac{\partial^2 \omega_j^2(\underline{k})}{\partial k_i \partial k_j} \Bigg|_{\underline{k} = \underline{k}_o^j} \qquad \text{(AII-9)}$$

One can similarly expand $\lambda_{\mu\nu}(\underline{k})$ around $\underline{k}_o^j$, but only the $\lambda_{\mu\nu}(\underline{k}_o^j)$ term will give a significant contribution because the higher terms will ultimately lead to terms of the order of $\frac{1}{R^3}$ which will be negligible when R is large. Further if there are more than one $(\underline{k}_o^j, t_o)$ that satisfy equation (AII-6) then a summation must be done over all of them.

Thus equation (AII-4) can be written as

$$I(\underline{R},\omega) = \sum_{\text{all } \underline{k}_o^j, t_o} e^{i\,\underline{k}_o^j\cdot\underline{R}}\, \lambda_{\mu\nu}(\underline{k}_o^j)\; i\int d\tau \iiint d^3K \exp^{-i}\Big[\tau\sum_i \beta_i K_i + t_o \sum_{i,j}\alpha_{ij}K_iK_j\Big] \qquad \text{(AII-10)}$$

This can be further simplified by writing the phase in matrix and vector notation as

$$\tau\sum_i \beta_i K_i + t_o \sum_{i,j}\alpha_{ij}K_iK_j = \tau\underline{\beta}^T\underline{K} + t_o\underline{K}^T\hat{\alpha}\,\underline{K}$$

where T denotes the transpose.

Further if we define $\underline{p} = \underline{K} + \frac{1}{2}\frac{\tau}{t_o}\hat{\alpha}^{-1}\underline{\beta}$

then

$$\tau\underline{\beta}\cdot\underline{K} + t_o\underline{K}^T\hat{\alpha}\,\underline{K} = -\frac{1}{4}\,\frac{\tau^2}{t_o}\,\underline{\beta}^T\hat{\alpha}^{-1}\underline{\beta} + t_o\,\underline{p}^T\hat{\alpha}\,\underline{p}$$

and $d^3K = d^3p$. We have used the fact that $\hat{\alpha}$ is symmetric which is obvious from its definition. Substituting this in equation (AII-10), we get

$$I(\underline{R},\omega) = \sum_{\text{all } \underline{k}_o^j, t_o} e^{i\underline{k}_o^j\cdot\underline{R}}\, \lambda_{\mu\nu}(\underline{k}_o^j)\; i\int d\tau\; e^{\frac{i}{4t_o}\tau^2\underline{\beta}^T\hat{\alpha}^{-1}\underline{\beta}} \iiint d^3p\; e^{-it_o\underline{p}^T\hat{\alpha}\,\underline{p}}$$

$$= \sum_{\text{all } \underline{k}_o^j, t_o} e^{i\,\underline{k}_o^j\cdot\underline{R}}\, \lambda_{\mu\nu}(\underline{k}_o^j)\; i\int d\tau\; e^{\left(\frac{i}{4t_o}\underline{\beta}^T\hat{\alpha}^{-1}\underline{\beta}\right)\tau^2} \times \sqrt{\pi^3}\Big/\sqrt{\left(i\,t_o^3\det|\hat{\alpha}|\right)}$$

where the limits of p integration is extended to ± ∞. Extending the limits of τ integration similarly, one obtains

$$I(\underline{R},\omega) = \sum_{\text{all } \underline{k}_o^j, t_o} e^{i\underline{k}_o^j \cdot \underline{R}} \lambda_{\mu\nu}(\underline{k}_o^j)\, i \sqrt{\frac{\pi}{\frac{i}{4t_o}\underline{\beta}^T \hat{\alpha}^{-1} \underline{\beta}}} \times \sqrt{\frac{\pi^3}{i t_o^3 \det|\hat{\alpha}|}}$$

$$= \sum_{\text{all } \underline{k}_o^j, t_o} e^{i\underline{k}_o^j \cdot \underline{R}} \lambda_{\mu\nu}(\underline{k}_o^j) \frac{2\pi^2}{t_o \sqrt{\underline{\beta}^T \hat{\alpha}^{-1} \underline{\beta} \det|\hat{\alpha}|}}$$

(AII-11)

But from equations (AII-6) and (AII-8) one has

$$\beta_i = \frac{R_i}{t_o} \quad \text{whence } t_o = \frac{\sqrt{\beta_i^2}}{R} = \frac{\sqrt{\underline{\beta}^T \underline{\beta}}}{R}$$

Hence

$$I(\underline{R},\omega) = \sum_{\text{all } \underline{k}_o^j} 2\pi^2 \frac{e^{i\underline{k}_o^j \cdot \underline{R}}}{R} \lambda_{\mu\nu}(\underline{k}_o^j) \frac{\sqrt{\underline{\beta}^T \underline{\beta}}}{\sqrt{\underline{\beta}^T \hat{\alpha}^{-1} \underline{\beta} \det|\hat{\alpha}|}}$$

(AII-12)

Putting this in equation (AII-3) one gets the final form as

$$G^j_{\mu\nu}(\omega^2, \underline{R}) = \frac{-2\pi^2}{MV^*} \sum_{\text{all } \underline{k}_o^j} \frac{\exp(i\underline{k}_o^j \cdot \underline{R})}{R} \lambda_{\mu\nu}(\underline{k}_o^j) \times \sqrt{\frac{\underline{\beta}^T \underline{\beta}}{\left[\underline{\beta}^T \hat{\alpha}^{-1} \det|\hat{\alpha}|\, \underline{\beta}\right]}} \quad \text{(AII-13)}$$

Now for the scalar models, the branch index j can be omitted and comparing equation (AII-2) with the corresponding equation of the scalar models described in equation (AI-1) one finds that $\lambda_{\mu\nu}(\underline{k})$ is unity. Thus for the simple cubic, body centred cubic and face centred cubic scalar models one obtains

$$C_{S,B,F}(\omega^2, \underline{R}) = -\sum_{\text{all } k_o} g_{S,B,F}(\underline{k}_o) \frac{\exp(i\underline{k}_o \cdot \underline{R})}{R} \qquad \text{(AII-14)}$$

where evaluating β_i and α_{ij}, as defined by equations (AII-8) and (AII-9) we get

$$g_S(\underline{k}_o) = \frac{1}{4\pi\gamma}\left[\frac{\sin^2 k_{o1} + \sin^2 k_{o2} + \sin^2 k_{o3}}{\sin^2 k_{o1}\cos k_{o2}\cos k_{o3} + \sin^2 k_{o2}\cos k_{o3}\cos k_{o1} + \sin^2 k_{o3}\cos k_{o1}\cos k_{o2}}\right]^{\frac{1}{2}}$$

(AII-15)

$$g_B(\underline{k}_o) = \frac{1}{8\pi\gamma}\left[\frac{S_1^2C_2^2C_3^2 + S_2^2C_3^2C_1^2 + S_3^2C_1^2C_2^2}{C_1^2C_2^2C_3^2(S_1^2+S_2^2+S_3^2)}\right]^{\frac{1}{2}} \qquad \text{(AII-16)}$$

where $C_i = \cos \tfrac{1}{2}k_{oi}$ and $S_i = \sin \tfrac{1}{2}k_{oi}$.

For face centred cubic

$$g_F(\underline{k}_o) = \frac{1}{8\pi\gamma}\left[\frac{S_1^2(C_2+C_3)^2 + S_2^2(C_3+C_1)^2 + S_3^2(C_1+C_2)^2}{4S_1^2S_2^2S_3^2(C_1C_2+C_2C_3+C_3C_1)+(C_1+C_2)(C_2+C_3)(C_3+C_1) \times \left\{S_1^2(C_2+C_3)+S_2^2(C_3+C_1)+S_3^2(C_1+C_2)\right\}}\right]^{\frac{1}{2}} \qquad \text{(AII-17)}$$

For those scalar models, not more than one $\underline{k}_o$ is obtained as solution of equation (AII-6) in the limit of long waves because the constant frequency surfaces are spherical in this limit for these models. So the summation over $\underline{k}_o$ is to be omitted. We have omitted this summation also in other cases where we are not interested in finding out numbers or exact results but require only qualitative aspects of the results.

For the case of the model with polarization

$\lambda_{\mu\nu}(\underline{k}) = e^{*(j)}_{\mu}(\underline{k})\, e^{(j)}_{\nu}(\underline{k})$ where $e^{(j)}_{\mu}(\underline{k})$ is the μ th component of the jth polarization vector. Then one gets

$$G_{\mu\nu}(\omega^2;\underline{R}) = -\sum_{j}\sum_{\text{all } \underline{k}_o^j} e^{(j)}_{\mu}(\underline{k}_o^j)\, g_{\nu}(\underline{k}_o^j)\, \exp(i\underline{k}_o^j.\underline{R})\ /R \tag{AII-18}$$

where

$$g_{\nu}(\underline{k}_o^j) = \frac{2\pi^2\, e^{*(j)}_{\nu}(\underline{k}_o^j)}{MV^*}\sqrt{\frac{\underline{\beta}^T\underline{\beta}}{\underline{\beta}^T\hat{\alpha}^{-1}\det|\hat{\alpha}|\underline{\beta}}} \tag{AII-19}$$

The vector $\underline{\beta}$ and the matrix $\hat{\alpha}$ in equation (AII-19) have to be evaluated at $\underline{k}_o^j$.

...

APPENDIX III

EVALUATION OF $\hat{V}$ - MATRICES

Consider a lattice whose symmetry point group consists of elements $\{R\}$ with the corresponding operations O_R. Let N_g be the order of the group and let there be h irreducible representations $\Gamma^{(\nu)}, \nu = 1, \ldots, h$, of this group. We denote the dimensionality of the irreducible representation $\Gamma^{(\nu)}$ by n_ν and the unitary matrices corresponding to operations O_R in this irreducible representation by $\hat{D}^{(\nu)}(R)$ whose traces or characters are given by $\chi^{(\nu)}(R)$. In addition to this point group of symmetry, the lattice has translational invariance but this is destroyed when we put in a substitutional impurity and we assume that the system still has this point group symmetry. The displacements of the substitutional impurity and its neighbours form a space S which is invariant under the group of unitary operators $\{O_R\}$. The characters $\chi(R)$ of this space S with respect to the group can be found and then the representation Γ of the group in the space S can be written as,

$$\Gamma = \sum_\nu a_\nu \Gamma^{(\nu)} \qquad \text{(A III -1)}$$

where[42]

$$a_\nu = \frac{1}{N_g} \sum_R \chi(R) \chi^{(\nu)*}(R) \qquad \text{(A III - 2)}$$

This shows that the space S can be split into irreducible subspaces $S^{(\nu)}$ which occur a_ν times for a given ν. If there is a non-zero vector ψ in the space S then the operators,

$$P^{(\nu)}_{rs} = \frac{n_\nu}{N_g} \sum_R D^{(\nu)*}_{rs}(R) \; O_R \qquad \text{(A III-3)}$$

project out those vectors in the space S that belong to the rth

row of the ν^{th} irreducible representation of the group.[49] This is subject to the condition that $P^{(\nu)}_{rs}\,\psi$ is not identically equal to zero.

Since $\hat{D}^{(\nu)}$ are $n_\nu \times n_\nu$ matrices, there are in all $\sum_{\nu=1}^{h} n_\nu^2 = N_g$ such projection operators. Using these we can form the different symmetry adapted vectors out of ψ . It is to be noted that the choice of ψ is completely arbitrary and it is a matter of convenience. By varying r,s and ν , we arrive at vectors that have the symmetries of different irreducible representations. These are orthogonal to one another and with proper normalisation they constitute the columns of the required $\hat{V}$ matrix, which block diagonolizes the matrices $\hat{p}$ and $\hat{g}$. This block diagonolization follows the properties of these column vectors and from the fact that the operators O_R commute with $\hat{p}$ and $\hat{g}$.

We consider the specific case of the cubic group O_h whose order $N_g = 48$ and whose character table is depicted in table III below in the notation of Hamermesh[42] . Using equation (A III-3) for the simple cubic, body centred cubic , face centred cubic and the polarization model, which are denoted by the subscripts S, B, F and P respectively, one gets with the aid of table III,

$$\Gamma_S = 2\,A_{1g} + F_{1u} + E_g$$

$$\Gamma_B = 2\,A_{1g} + F_{1u} + F_{2g} + A_{2u}$$

$$\Gamma_F = 2\,A_{1g} + F_{1u} + E_g + F_{2g} + F_{2u}$$

$$\Gamma_P = F_{1u} \otimes (2\,A_{1g} + F_{1u} + F_{2g} + A_{2u})$$

where $\otimes$ denotes the direct product of the irreducible representations.

TABLE III

CHARACTER TABLE FOR O_h

Representations.	Notation[9,20]	E	$8C_3$	$3C_4^2$	$6C_2$	$6C_4$	I	$8S_6$	$3\sigma_h$	$6\sigma_d$	$6S_4$
A_{1g}	S	1	1	1	1	1	1	1	1	1	1
A_{1u}	L	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2g}	I	1	1	1	-1	-1	1	1	1	-1	-1
A_{2u}	F_1	1	1	1	-1	-1	-1	-1	-1	1	1
E_g	D_1	2	-1	2	0	0	2	-1	2	0	0
E_u	H	2	-1	2	0	0	-2	1	-2	0	0
F_{1g}	G	3	0	-1	-1	1	3	0	-1	-1	1
F_{1u}	P	3	0	-1	-1	1	-3	0	1	1	-1
F_{2g}	D_2	3	0	-1	1	-1	3	0	-1	1	-1
F_{2u}	F_2	3	0	-1	1	-1	-3	0	1	-1	1
Γ_S		7	1	3	1	3	1	1	5	3	1
Γ_B		9	3	1	1	1	1	1	1	5	1
Γ_F		13	1	1	3	1	1	1	5	3	1
Γ_P		27	0	-1	-1	1	-3	0	1	5	-1

The matrices $\hat{D}(\nu)$ are worked out using the basis given in Hamermesh[42], for example. Now following the procedure described we arrive at the following forms of $\hat{V}$ - matrices. In these, for each irreducible representation of dimensionality n_α appearing once in the reduced form of Γ, one has n_α columns.. If it appears a_α times then one has $a_\alpha \times n_\alpha$ columns.

The elements of $\hat{V}$-matrices given below are given in terms of numerical quantities given by ,

$$b = (8)^{-\frac{1}{2}} ,\; c = (24)^{-\frac{1}{2}},\; d = \tfrac{1}{2} ,\; h = (12)^{-\frac{1}{2}},\; d' = (6)^{-\frac{1}{2}} \text{ and } h' = (2)^{-\frac{1}{2}}$$

(i) For the simple cubic lattice we get ,

$$\hat{V}_S = \begin{array}{c}\left(\begin{array}{ccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & d' & h' & 0 & 0 & h & d \\ 0 & d' & 0 & h' & 0 & h & -d \\ 0 & d' & 0 & 0 & h' & -2h & 0 \\ 0 & d' & -h' & 0 & 0 & h & d \\ 0 & d' & 0 & -h' & 0 & h & -d \\ 0 & d' & 0 & 0 & -h' & -2h & 0 \end{array}\right) \\ \underbrace{\qquad\quad}_{2A_{1g}} \quad \underbrace{\qquad\qquad\qquad}_{F_{1u}} \quad \underbrace{\qquad\quad}_{E_g} \end{array} \qquad (4\ \text{III-4})$$

Here the row and column indices, starting from upper left corner are (0,0,0) , (1,0,0) , (0,1,0) , (0,0,1) , (-1,0,0) , (0,-1,0) and (0,0,-1) where the numbers refer to (l ,m,n) values for the nearest neighbour sites according to equation (3.1) of chapter III.

(ii) For the body centred cubic lattice, we have

$$\hat{V}_B = \begin{array}{c}\left(\begin{array}{ccccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b & b & b & b & b & b & b & b \\ 0 & b & b & -b & b & b & -b & -b & -b \\ 0 & b & -b & -b & b & -b & -b & b & b \\ 0 & b & -b & b & b & -b & b & -b & -b \\ 0 & b & -b & -b & -b & b & b & b & -b \\ 0 & b & -b & b & -b & b & -b & -b & b \\ 0 & b & b & b & -b & -b & -b & b & -b \\ 0 & b & b & -b & -b & -b & b & -b & b \end{array}\right) \\ \underbrace{\qquad\quad}_{2\ A_{1g}} \quad \underbrace{\qquad\qquad\qquad}_{F_{1u}} \quad \underbrace{\qquad\qquad\qquad}_{F_{2g}} \quad \underbrace{\quad}_{A_{2u}} \end{array} \qquad (\text{AIII-5 })$$

with the row and column indices starting from the upper left corner as (0,0,0),(0,1,0), (1,-1,0) , (0,-1,1) , (-1,1,-1), (0,-1,0) ,(-1,1,0), (0,1,-1) and (1,-1,1) , the numbers here referring to the (l ,m,n) values for the nearest neighbour sites according to equations (4.1).

(iii) and for the face centred cubic lattice,

$$\hat{V}_F = \begin{array}{c} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h & b & 0 & b & b & c & d & 0 & 0 & b & b & 0 \\ 0 & h & b & 0 & -b & b & c & -d & 0 & 0 & -b & b & 0 \\ 0 & h & b & b & 0 & 0 & -2c & 0 & d & 0 & 0 & -b & b \\ 0 & h & b & -b & 0 & 0 & -2c & 0 & -d & 0 & 0 & -b & -b \\ 0 & h & 0 & b & -b & -b & c & 0 & 0 & d & b & 0 & -b \\ 0 & h & 0 & b & b & -b & c & 0 & 0 & -d & -b & 0 & -b \\ 0 & h & -b & 0 & -b & b & c & d & 0 & 0 & -b & -b & 0 \\ 0 & h & -b & 0 & b & b & c & -d & 0 & 0 & b & -b & 0 \\ 0 & h & -b & -b & 0 & 0 & -2c & 0 & d & 0 & 0 & b & -b \\ 0 & h & -b & b & 0 & 0 & -2c & 0 & -d & 0 & 0 & b & b \\ 0 & h & 0 & -b & b & -b & c & 0 & 0 & d & -b & 0 & b \\ 0 & h & 0 & -b & -b & -b & c & 0 & 0 & -d & b & 0 & b \end{pmatrix} \\ \underbrace{\qquad}_{2A_{1g}} \qquad \underbrace{\qquad\qquad\qquad}_{F_{1u}} \qquad \underbrace{\qquad\quad}_{E_g} \qquad \underbrace{\qquad\qquad\quad}_{F_{2g}} \qquad \underbrace{\qquad\qquad\quad}_{F_{2u}} \end{array} \qquad \text{(AIII-6)}$$

with the row and column indices starting from the upper left corner as (0,0,0) , (1,0,0) , (0,1,-1) , (0,1,0) , (1,0,-1) , (-1,1,0) ,(0,0,1) (-1,0,0) , (0,-1,1) , (0,-1,0), (-1,0,1) , (1,-1,0) and (0,0,-1) .

Finally the matrix $\hat{V}_P$ for the model with polarization is a 27 x 27 matrix which can be partitioned into 9 x 9 submatrices as shown in equation (5.53) of chapter V.

$$\hat{V}_P = \begin{pmatrix} \hat{V}_{11} & \hat{V}_{12} & \hat{V}_{13} \\ \hat{V}_{21} & \hat{V}_{22} & \hat{V}_{23} \\ \hat{V}_{31} & \hat{V}_{32} & \hat{V}_{33} \end{pmatrix} \qquad \text{(AIII-7)}$$

Each of those submatrices have row and column indices the same as described for $\hat{V}_B$ above (equation (AIII-5)). The order of columns of $\hat{V}_P$ will correspond to the following order of the irreducible representations of O_h appearing in the reduced form of Γ_P .

$$3F_{1u} \ , \ A_{1g} \ , \ E_g \ , \ 2F_{2g} \ , \ A_{2u} \ , \ F_{2u} \ , \ F_{1g} \text{ and } E_u \ .$$

This leads to the order of blocks described in chapter V.

Explicitly, the matrices $\hat{V}_{ij}$,(i,j = 1,2,3) of equation (AIII-7) can be written by using the following nine dimensional vectors.

$$X_0 = \begin{bmatrix} 0\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}, X_1 = \begin{bmatrix} 1\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}, X_2 = \begin{bmatrix} 0\\b\\b\\b\\b\\b\\b\\b\\b \end{bmatrix}, \psi_3 = \begin{bmatrix} 0\\1\\1\\-1\\-1\\-1\\-1\\1\\1 \end{bmatrix}, \psi_4 = \begin{bmatrix} 0\\1\\-1\\-1\\1\\-1\\1\\1\\-1 \end{bmatrix}, \psi_5 = \begin{bmatrix} 0\\1\\1\\1\\1\\-1\\-1\\-1\\-1 \end{bmatrix}$$

$$\psi_6 = \begin{bmatrix} 0\\1\\1\\-1\\-1\\1\\1\\-1\\-1 \end{bmatrix}, \psi_7 = \begin{bmatrix} 0\\1\\-1\\-1\\1\\1\\-1\\-1\\1 \end{bmatrix}, \psi_8 = \begin{bmatrix} 0\\1\\-1\\1\\-1\\1\\-1\\1\\-1 \end{bmatrix} \text{ and } X_9 = \begin{bmatrix} 0\\b\\-b\\b\\-b\\-b\\b\\-b\\b \end{bmatrix}$$

and defining the vectors,

$$X_i = (\psi_i)/4\ ,\ Y_i = c\psi_i\ ,\ Z_i = bd'\psi_i \text{ for } i = 3,4,\ \ldots,8$$

By writing these vectors side by side with appropriate factors and signs , the submatrices $\hat{V}_{ij}$ are,

$$V_{11} = (X_1 \quad X_2 \quad X_0 \quad X_0 \quad X_0 \quad X_8 \quad X_0 \quad X_0 \quad X_7\ )$$

$$V_{12} = (Y_4 \quad X_4 \quad Z_4 \quad X_3 \quad X_0 \quad X_5 \quad X_0 \quad X_0 \quad X_9\ )$$

$$V_{13} = (Y_6 \quad X_7 \quad X_0 \quad X_8 \quad X_0 \quad X_5 \quad X_3 \quad Z_6 \quad X_6\ )$$

$$V_{21} = (X_0 \quad X_0 \quad X_8 \quad X_1 \quad X_2 \quad X_0 \quad X_0 \quad X_0 \quad X_6\ )$$

$$V_{22} = (Y_3 \quad -X_3 \quad Z_3 \quad X_4 \quad X_0 \quad X_0 \quad X_9 \quad X_5 \quad X_0\ )$$

$$V_{23} = (Y_7 \quad -X_6 \quad -X_8 \quad X_0 \quad -X_5 \quad X_0 \quad -X_4 \quad Z_7 \quad -X_7\ )$$

$$V_{31} = (X_0 \quad X_0 \quad X_7 \quad X_0 \quad X_0 \quad X_6 \quad X_1 \quad X_2 \quad X_0\ )$$

$$V_{32} = (Y_5 \quad X_0 \quad -2Z_5 \quad X_0 \quad X_9 \quad X_4 \quad X_0 \quad X_3 \quad X_0\ ) \quad \text{and}$$

$$V_{33} = (Y_8 \quad X_0 \quad X_7 \quad -X_6 \quad X_3 \quad -X_4 \quad X_0 \quad -2Z_8 \quad X_0\ )$$

When all these are put together in equation (AIII-7) one gets the full 27 x 27 matrix $\hat{V}_P$ which is used in chapter V.

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